Appendix 3

8-Hour Ozone Modeling Analysis and Attainment Demonstration For South Carolina's Early Action Compact

Technical Protocol

D H E C

PROMOTE PROTECT PROSPER

Contents

1 INTRODUCTION AND MODELING ANALYSIS/ATTAINMENT DEMONSTRATION DESIGN

This protocol document outlines the methods and procedures to be followed in conducting 8-hour ozone modeling attainment demonstration for submittal to the Environmental Protection Agency (EPA) as part of the State of South Carolina and the South Carolina Department of Health and Environmental Control's (SC DHEC) Early Action Plan Compact for ozone. This regional-scale modeling analysis will provide technical information relevant to attainment of an 8-hour National Ambient Air Quality Standard (NAAQS) for ozone in South Carolina, with emphasis on the Anderson/Greenville/Spartanburg, Aiken/Columbia, Darlington/Florence, and Rock Hill areas. Information obtained through modeling is intended to provide the basis for attainment demonstration for each of the areas. The protocol document was prepared based on draft EPA guidance (EPA, 1999a) on the use of models and other analyses to demonstrate attainment of the 8-hour NAAQS at the 0.80 parts per million (ppm) level.

This modeling demonstration is based on the 8-hr ozone modeling contract through SAI for SC DHEC which began in early 2001. This work is nearly complete and will provide a 1998 base-case and a 2010 future-year case. The protocol prepared by SAI for this initial modeling has been revised by SC DHEC to incorporate the necessary changes needed for an attainment demonstration under it's Early Action Compact.

Information regarding the organizational structure of the SC DHEC modeling analysis, modeling analysis participants, communication structures, and the resolution of technical difficulties is presented in this section. The goals, objectives, and technical components of the modeling/analysis are briefly described. Issues related to the demonstration protocol are discussed and a schedule is provided.

Please note that this protocol document addresses the full attainment demonstration modeling analysis, by component. Episode selection was conducted by SC DHEC and reviewed/finalized by Systems Applications International, Inc. (SAI). The 1998 base-case and 2010 future-year baseline modeling were conducted primarily by SAI, under contract to the State of South Carolina. SAI has also been contracted to develop 2007 and 2012 future-year inventories for SC DHEC. The sensitivity and control-strategy runs will be conducted by SC DHEC with assistance from SAI as needed. The procedures for these components of the modeling analysis are presented in some detail and are not expected to vary much throughout this phase of the attainment demonstration. The sensitivity and future-year control-strategy modeling and the attainment demonstration will be conducted primarily by SC DHEC with assistance from SAI as needed; the procedures presented in the protocol document for this phase of the attainment demonstration may evolve based on the modeling results and in response to changes in the EPA requirements for 8-hour ozone modeling attainment demonstrations.

Please note that the number of days in the attainment demonstration modeling analysis is five plus two startup and one cleanout day. SC DHEC realizes that is less than the currently recommended number of ten days for an attainment test. When we started this project the draft 8-hr Modeling Guidance was silent on the number of days needed for an attainment demonstration. It did mention the ten days in relation to Figure 3.3 in the guidance. However, no mention was made of having to use ten days in order to apply the test. The guidance only mentioned that several days should be used. In fact the example episode used contained only four days. Also, the project was not initially intended to serve as an attainment demonstration. We intended to partner with NC on another episode and possibly run a third. However, NC halted work on their episode and the second episode did not become a reality. SC DHEC would like to participate in the Early Action Compact and we would not have enough time to complete another episode, since our administrative process requires us to submit the attainment SIP package to our Legislature for approval. This gives us less than 10 months total for the work to be completed. SC DHEC has been told by the EPA that their modeling work for various purposes have shown that our State will meet the 8-hr ozone standard from just the NOx SIP Call reductions and reductions from other national regulatory efforts, primarily in the mobile source area. We also understand that other modeling by NC has indicated the same thing. South Carolina will come back into attainment with just the reductions mentioned above. Therefore, SC DHEC requests that EPA accept our attainment demonstration modeling as submitted.

COMMITTEE COMPOSITION AND RESPONSIBILITIES

SC DHEC has established one committee and plans to establish a second committee to help with the work involved in this ozone demonstration, a policy committee composed of individuals from SC DHEC and the Clean Air Partnership, and a technical committee composed of persons with technical expertise from SC DHEC, the Clean Air Partnership, and other participating entities.

The policy committee will provide guidance on control scenarios to be run in the ozone model. This committee has not met yet.

The technical committee provides guidance on the work of the consultant. This broad-based committee of stakeholders with technical expertise meets regularly to discuss and take action on specific tasks to be completed by the contractor. These tasks may include, but are not limited to, procedures used to select episodes for modeling, development of appropriate emissions inventories, development of meteorological fields associated with the selected episodes, sensitivity runs of the photochemical grid model, control strategy runs for the photochemical grid model, and presentation of results. These tasks and others are contained in a previously completed work plan and more specifically outlined within this protocol. The technical committee may in its judgement add to these tasks, subject to the needs of the members of the committee and availability of funding. This committee has already been formed and has met on four occasions.

MODELING ANALYSIS PARTICIPANTS AND THEIR ROLES

SC DHEC is the principal participant in this modeling demonstration. The role of the principal participant is somewhat greater than that of the other participants. The principal participant funds the demonstration and plays a more direct role in the day-to-day operations and contact with the contractor. The principal participant makes final decisions on tasks and project management. The involvement of others is through their active participation on the technical committee.

The tasks mentioned earlier will be conducted by Systems Applications International, Incorporated (SAI) and SC DHEC. Jay Haney and Sharon Douglas will serve as project manager and technical coordinator, respectively, for SAI. Clay Lawson will serve as project manager for SC DHEC.

COMMUNICATIONS STRUCTURES

Communication among the participants occurs during bimonthly (approximately) face-to-face meetings of the participants in the technical aspects of the modeling analysis, biweekly (approximately) teleconferences of the technical committee, and continuous (as necessary) e-mail and telephone. A web site set up by the consultant contains information and results generated in the base-case modeling analysis. Future-year and control-strategy information and results will be posted to the SC DHEC web site.

Communication between the contractor and the participants will be through the contractor's participation in the face-to-face and teleconference meetings, and by an e-mail distribution list. Outside of these meetings, communication between the contractor and the participants will be from the members of the operations committee (project manager and designated members).

SAI will report directly to SC DHEC. Kevin Clark will serve as the project manager for SC DHEC.

RESOLUTION OF TECHNICAL DIFFICULTIES

Technical difficulties encountered by SAI will be brought to the attention of the SC DHEC project manager through written correspondence. SAI will also offer suggestions or recommendations on how to resolve such difficulties. All major issues or difficulties (whether or not they are fully or satisfactorily resolved during the course of the modeling analysis) will be documented, in either a technical memorandum or the modeling/analysis report.

GOALS AND OBJECTIVES OF THE MODELING ANALYSIS

The SC DHEC regional-scale modeling analysis is designed to provide technical information relevant to attainment of an 8-hour National Ambient Air Quality Standard (NAAQS) for ozone in South Carolina, with emphasis on the Anderson/Greenville/Spartanburg, Aiken/Columbia, Darlington/Florence, and Rock Hill areas. In addition, it provided technology transfer, training, and support in setting up and conducting planned future-year emission-reduction and/or control-strategy simulations. The above areas are likely to be included in designated nonattainment areas under a new 8-hour National Ambient Air Quality Standard (NAAQS) for ozone. This standard requires the three-year average of the fourth highest ozone concentration for a given monitoring site to be less than 85 parts per billion (ppb). Initial compliance with this standard was scheduled to be determined using data collected during the period 1997-1999. Based on data for 1997-1999, the 1998 design values for the areas listed above are given in Table 1-1.

TABLE 1-1. 1997-1999 8-hour ozone "design values" for the South Carolina areas of interest.

Area	1997-1999 Design Value (ppb)
Anderson/Greenville/Spartanburg	95
Aiken/Columbia	92
Darlington/Florence	88
Rock Hill	86

Also of interest are the 2000-2002 design values for the areas of interest as given in Table 1-2. These will also be used in the application of the modeled attainment test, as described later in this protocol document.

TABLE 1-2. 2000-2002 8-hour ozone "design values" for the South Carolina areas of interest.

Area	2000-2002 Design Value (ppb)
Anderson/Greenville/Spartanburg	90
Aiken/Columbia	88
Darlington/Florence	86
Rock Hill	84

A designation of nonattainment relative to the 8-hour ozone standard requires that air quality modeling techniques be applied as part of an attainment demonstration. Thus, the primary objective of this modeling analysis is to provide the data needed to support an attainment demonstration for each of these areas. As such, the attainment demonstration has been designed in accordance with draft EPA guidance (EPA, 1999a) for using modeling and other analyses for 8-hour ozone attainment demonstration purposes. Note that while the guidance is currently in draft form, the final version is not expected to be substantively different from the draft (EPA, personal communication). Changes by EPA in its expectations for ozone modeling will be addressed via modifications in the protocol and/or the workplan.

The results of this modeling analysis/attainment demonstration will be presented in a single report, with separate sections for the presentation of results for each area of interest. The analytical results will also be presented in electronic/database format such that each of the areas can be examined separately. They will then be referenced into State Implementation Plan (SIP) documentation prepared by SC DHEC as part of its Early Action Compact.

MODELING/ANALYSIS COMPONENTS

The SC DHEC modeling analysis components include a comprehensive episode selection analysis (identifying suitable periods for modeling), application and evaluation of a photochemical modeling system for one simulation period, projection of emissions and ozone concentrations for one or more future years, and evaluation of ozone attainment strategies. While photochemical modeling is currently the best available and most widely used technique to estimate the effects of emission changes on future-year ozone air quality and to evaluate attainment strategies, EPA also recommends (EPA, 1999a) that additional analysis of observational data be included as part of an attainment demonstration. Thus it is anticipated that future efforts may also include the analysis of observational data to corroborate the results and conclusions of the modeling analysis. All technical tasks will be conducted in accordance with draft EPA guidance regarding the use of modeling and other analyses for 8-hour ozone attainment demonstration (EPA, 1999a). The documentation prepared as part of this modeling analysis/attainment demonstration will be referenced by the SIP for SC DHEC's Early Action Compact.

PROTOCOL OBJECTIVES, CONTENTS, AND AMENDMENT PROCEDURES

This protocol document should be viewed as a set of general guidelines and is intended to provide focus, consistency, and a basis for consensus for all parties involved in the modeling analysis.

The primary purpose of the protocol document is to outline the methodologies to be followed throughout the modeling analysis/attainment demonstration. At this time some of the methodologies to be used in the modeling analysis/attainment demonstration have not been finalized. It will be necessary for the attainment demonstration participants to make decisions regarding these issues as the attainment demonstration progresses. Amendment of the protocol document will occur only upon the direction of SC DHEC. Each time the protocol document is amended, a revised version of the entire document will be made available in electronic format on SC DHEC's web site.

The remainder of this document provides detailed information on each element of the modeling analysis. Selection of the primary modeling tools is summarized in Section 2 and a brief overview of each is provided. The methods and results of the episode selection analysis are provided in Section 3. The modeling domain is presented in Section 4. Model input preparation procedures are described in Section 5. Model performance evaluation is discussed in Section 6. The use of diagnostic and sensitivity analysis is outlined in Section 7. Future-year modeling is discussed in Section 8. A description of the attainment demonstration procedures is given in Section 9. Documentation procedures are detailed in Section 10. The deliverables and schedule for the project are summarized in Section 11. Archival and data acquisition procedures are outlined in Section 12.

SCHEDULE

A schedule for base-case and future-year baseline components of the SC DHEC modeling analysis is provided below:

December 31, 2002 - Base-case modeling complete

April 30, 2003 - Future-year inventories completed by consultant

October 31, 2003 - Modeling completed for 2007 future-year case

January 31, 2004 - Modeling completed for at least one control-strategy case.

March 31, 2004 - All modeling completed and report finalized

2 MODEL SELECTION

The selection of modeling tools for this study considered (1) technical formulation, capabilities, and features, (2) comprehensiveness of testing, and (3) demonstrated successful use in previous applications (similar in scope to the South Carolina 8-hour ozone modeling analysis). The primary modeling tools selected for use in this study include: the variable-grid Urban Airshed Model (UAM-V), a regional-scale, nested-grid photochemical model; an enhanced version of EPA's Emissions Preprocessing System (EPS2.5), for preparation of model-ready emission inventories; the latest available version of EPA's Biogenic Emission Inventory System (BEIS), for estimating biogenic emissions; the latest available version of the EPA MOBILE6 model; and the latest available PSU/NCAR Mesoscale Model, Version 5 (MM5), for preparation of the meteorological inputs. The rationale for selecting each of these modeling tools (in keeping with EPA guidance) is discussed in this section; an overview of each modeling tool is also provided.

The modeling tools to be used for this project must be capable of being upgraded to all modeling of fine particulate matter (PM). In this regard, UAM-V and EPS2.5 are also excellent choices. UAM-V is currently being upgraded to include state-of-the science PM chemistry. A description of UAM-VPM is given later in this section. Except for an additional input file and some added species in the emissions inventory, the databases prepared for this project will be suitable for use with UAM-VPM. The EPS2.5 emissions processing programs already support the preparation of emissions for PM modeling; this tool has been used to prepare inputs for the REgulatory Modeling System for Aerosols and Deposition for several recent applications. As an alternative to UAM-VPM, the input files (with some minor adjustments) can also be used in the application of REMSAD.

SELECTION AND OVERVIEW OF THE PHOTOCHEMICAL MODEL

The UAM-V modeling system (Version 1.30) has been selected for use in this modeling study. The UAM-V is a state-of-the-science photochemical modeling system that incorporates the latest version of the Carbon-Bond IV (CB-IV) chemical mechanism with enhanced isoprene chemistry (Whitten et al., 1996) and a detailed treatment of selected hydrocarbon species and toxics (Ligocki and Whitten, 1992). This latter update to the chemical mechanism was implemented and tested during 1999 to improve the accuracy of the response of the modeling system to emission reductions under low hydrocarbon-to-NO_x ratio (hydrocarbon-limited) conditions. As a result, the mechanism is expected to yield more reliable results within urban areas, where hydrocarbon-limited conditions typically occur. Implementation of this enhancement involved the addition of two new carbon-bond categories for hydrocarbons (for higher aldehydes and internal olefins). Thus, simulation of the effects of control-strategies involving motor vehicle emissions (and other sources that emit these pollutant species) is expected to be more accurate. This is a key modeling-system strength when considering its use for the selected, moderately sized urban areas in South Carolina, where motor vehicles comprise a significant fraction of the emissions sources. Other models utilizing the CB-IV chemical mechanism do not have this latest enhancement. As an added benefit, the modeling system and databases, could also be easily used in the future to study toxics.

The UAM-V modeling system is designed for the regional-scale simulation of the physical and chemical processes that determine the spatial and temporal distribution of ozone and precursor pollutants within the atmospheric boundary layer. In addition to the enhanced chemical mechanism, other key features (strengths) of the UAM-V modeling system that are relevant to its use in this study include multiple nested-grid capabilities, ability to explicitly incorporate output from a dynamic meteorological model, a detailed plume-in-grid (P-i-G) treatment for emissions from elevated point sources, and the accommodation of process-level analysis of the simulation results.

The UAM-V modeling system is currently the most widely used and comprehensively tested photochemical modeling system in the world and its utility for both regional- and urban-scale analysis has been successfully demonstrated in dozens of applications (e.g., regional-scale modeling of the eastern U.S. as part of the Ozone Transport Assessment Group (OTAG) modeling study, SIP modeling of the Atlanta ozone nonattainment area by the Georgia Department of Natural Resources, SIP modeling of the Birmingham area by the Alabama Department of Environmental Management, SIP modeling of the Lake Michigan area by the Lake Michigan Air Directors Consortium). The UAM-V model is also currently being used for the Gulf Coast Ozone Study (GCOS), the Arkansas-Tennessee-Mississippi Ozone Study (ATMOS), SIP modeling for 1-hour ozone for Baton Rouge (Louisiana), and by EPA for analysis of the effects of Tier II motor-vehicle standards and other regional- and national-scale analysis of regulatory programs. Compared to other models that could be used for this study, the UAM-V model represents the most comprehensively tested photochemical modeling tool (for both research and regulatory purposes). It has been peer reviewed and used extensively by numerous organizations and for a variety of regions and air quality conditions in the U.S. and abroad. It is currently being employed by more than 100 agencies/organizations worldwide. Please refer to the UAM-V web site located at http:\\uamv.saintl.com for more information and a list of user countries.

EPA (1999a) list five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem**. High 8-hour ozone concentrations in the Anderson/Greenville/Spartenburg, Aiken/Columbia, Florence/Darlington, and Rock Hill areas are likely the combined result of local and regional influences (meteorology and emissions). The meteorology of South Carolina is generally favorable to low ozone concentrations. High ozone concentrations, however, occur under a variety of scenarios. Contributing factors include certain local meteorological conditions (e.g., high temperatures and light wind speeds – stagnation conditions associated with high pressure – can lead to local build up of ozone concentrations), regional-scale transport of ozone and precursor pollutants from nearby urban areas in North Carolina, Georgia, and/or other states, and the effects of the sea breeze in creating convergence zones and recirculating ozone and precursor pollutants within certain portions of the state. Emissions throughout the region and within the urban areas are from both low-level sources and elevated point sources. Thus the photochemical model to be used for this study should be capable of simulating the regional as well as the urban-scale processes associated with 8-hour ozone events, representing the complex meteorological features, and accurately incorporating emissions from a variety of sources.

The UAM-V modeling system is well suited for this application. The nested-grid feature will enable the use of large, intermediate, and high-resolution grids so that influences from other areas can be directly simulated, while the details of urban-scale ozone formation and transport over the areas of interest can be resolved. The model accommodates the use of detailed meteorological inputs from a dynamic meteorological model that will enable representation of the important mesoscale meteorological features such as the local airflow patterns, the sea breeze, temperature gradients, and vertical mixing patterns. The process-analysis feature of the UAM-V modeling system will enable an assessment of model performance at the process level and thus a comparison of the simulation results relative to conceptual models of ozone formation developed previously by DHEC and other researchers. Finally, the plume-in-grid (P-i-G) treatment available with UAM-V will accommodate the accurate simulation of emissions from elevated point sources and the interaction of these emissions with those from low-level sources.

- **Availability, documentation, and past performance should be satisfactory.** The UAM-V modeling system (Version 1.30), as proposed for this study, is available for free to all who request it. A user's group and a web site have recently been established to support its use by the more than 100 organizations that currently operate the UAM-V modeling system. From a Southeast regional perspective, the nearby/surrounding states of Georgia, Florida, Alabama, Mississippi, Louisiana, Tennessee, and Arkansas are currently using the UAM-V modeling system for their SIP modeling work. The UAM-V modeling system is fully documented, and has been demonstrated to perform satisfactorily in more than ten recent applications. Examples include the Atlanta SIP modeling, Baton Rouge SIP modeling, OTAG, the EPA-sponsored Section 812 prospective analysis, regional-scale modeling of the northeastern U.S. for assessment of the effects of urban-heat-island mitigation measures for EPA, regional-scale modeling of the Southeast (also used for the Birmingham SIP), and GCOS. Several additional references are provided in this section.

- **Relevant experience of available staff and contractors should be consistent with choice of a model.** SAI staff who have developed and are knowledgeable and experienced in the application of the UAM-V modeling system will perform the base-case and future-year baseline modeling tasks. All together, the SAI staff members proposed for this study have used the model in more than 100 studies/projects during the past eight years (since its development). They will bring the knowledge and experience from these studies to the South Carolina 8-hour ozone application. Transfer of the modeling tools and databases as well as training/instruction in their use will position SC DHEC to conduct additional future-year modeling exercises.

- **Time and resource constraints may be considered.** Given the demonstrated reliability of the model and the experience of the proposed staff, use of the UAM-V modeling system is consistent with the proposed schedule and costs.

- **Consistency of the model with what was used in adjacent regional applications should be considered.** The UAM-V modeling system was the photochemical model used for the OTAG regional-scale modeling effort. It has been used by the Texas Natural Resources Conservation Commission and the Tennessee Valley Authority for regional- or subregional modeling of their respective areas. It was also used by the Minerals Management Service (MMS) for modeling of the effects of emissions from offshore oil and gas production on the Gulf Coast area (Haney et al., 1995), a study explicitly called for in the Clean Air Act Amendments of 1990. The modeling system has been and/or is currently being used for regional-scale and SIP modeling of the Atlanta, Birmingham, and Baton Rouge areas. The UAM-V is also currently being used for 8-hour ozone assessment for the ATMOS modeling study (with emphasis on the Nashville, Knoxville, and Memphis areas) and the GCOS modeling study (with emphasis on Pensacola, Mobile, Pascagoula, Port Bienville, New Orleans, and Baton Rouge).

Overview of the UAM-V Modeling System

The variable-grid Urban Airshed Model (UAM-V) is a three-dimensional photochemical grid model that calculates concentrations of pollutants by simulating the physical and chemical processes in the atmosphere. The basis for the UAM-V is the atmospheric diffusion or species continuity equation. This equation represents a mass balance that includes all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes in mathematical terms.

The major factors that affect photochemical air quality include:

- pattern of emissions of NO_x and volatile organic compounds (VOC), both natural and anthropogenic

- composition of the emitted VOC and NO_x

- spatial and temporal variations in the wind fields

- dynamics of the boundary layer, including stability and the level of mixing

- chemical reactions involving VOC, NO_x, and other important species

- diurnal variations of solar insolation and temperature

- loss of ozone and ozone precursors by dry and wet deposition

- ambient background of VOC, NO_x, and other species in, immediately upwind of, and above the study region

The UAM-V simulates all of these processes. The species continuity equation is solved using the following fractional steps: emissions are injected; horizontal advection/diffusion are solved; vertical advection/diffusion and deposition are solved; and chemical transformations are performed for reactive pollutants. The UAM-V performs these four calculations during each time step. The maximum time step is a function of the grid size and the maximum wind velocity and diffusion coefficient. The typical time step is 10–15 minutes for coarse (10–20 km) grids and a few minutes for fine (2–4 km) grids.

Because it accounts for spatial and temporal variations as well as differences in the reactivity of emissions, the UAM-V is ideal for evaluating the air-quality effects of emission control scenarios. This is achieved by first replicating a historical ozone episode to establish a base-case simulation. Model inputs are prepared from observed meteorological, emissions, and air quality data for the episode days using prognostic meteorological modeling and/or diagnostic and interpolative modeling techniques. The model is then applied with these inputs, and the results are evaluated to determine model performance. Once the model results have been evaluated and determined to perform within prescribed levels, the same base-case meteorological inputs are combined with *modified* or *projected* emission inventories to simulate possible alternative/future emission scenarios.

The UAM-V modeling system incorporates the Carbon-Bond IV chemical mechanism with enhanced isoprene chemistry. It represents an extension of the UAM (also referred to as UAM-IV). Features of the UAM-V modeling system include:

1. *Variable vertical grid structure:* The structure of vertical layers can be arbitrarily defined. This allows for higher resolution near the surface and facilitates matching with output from prognostic meteorological models.

2. *Three-dimensional meteorological inputs:* The meteorological inputs for UAM-V vary spatially and temporally. These are usually calculated using a prognostic meteorological model.

3. *Variable grid resolution for chemical kinetic calculations:* A chemical aggregation scheme can be employed, allowing chemistry calculations to be performed on a variable grid while advection/diffusion and emissions injections are performed on a fixed grid.

4. *Two-way nested grid:* Finer grids can be imbedded in coarser grids for more detailed representation of advection/diffusion, chemistry, and emissions. Several levels of nesting can be accommodated.

5. *Updated chemical mechanism:* The original Carbon Bond IV chemical mechanism has been updated to include the XO_2–RO_2 reaction, new temperature effects for PAN reactions, enhanced isoprene chemistry, and more refined hydrocarbon speciation. Toxics are also an option.

6. *Process analysis capabilities:* The UAM-V process analysis technique allows a detailed inspection of the processes that determine the simulated ozone and precursor pollutant

concentrations including chemistry, horizontal advection, vertical advection, vertical diffusion, and deposition. This feature enhances the evaluation of model performance and interpretation and understanding of the response of the model to emission reductions.

7. *Dry deposition algorithm:* The dry deposition algorithm is similar to that used by the Regional Acid Deposition Model (RADM).

8. *True mass balance:* Concentrations are advected and diffused in the model using units of mass per unit volume rather than parts per million. This maintains true mass balance in the advection and diffusion calculations.

9. *Plume-in-grid treatment:* Emissions from point sources can be treated by a subgrid-scale Lagrangian photochemical plume model. Pollutant mass is released from the subgrid-scale model to the grid when the plume is commensurate with a grid cell size.

10. *Plume rise algorithm:* The plume rise algorithm is based on the plume rise treatment for a Gaussian dispersion model.

Acceptability Relative to the EPA Requirements

In accordance with EPA guidance (EPA, 1999a), use of the UAM-V modeling system for this study represents the use of an acceptable model for 8-hour ozone attainment demonstration purposes. While there is no "preferred" model identified in the guidance, EPA has used and continues to use the UAM-V for much of its modeling related to policy analysis (recent/current examples include modeling the effects of the of the NO_x SIP Call measures, assessment of the proposed Tier II motor-vehicle standards, examination of the costs and benefits of the 1990 Clean Air Act Amendments as part of the Section 812 prospective analysis, and analysis of the effects of urban-heat island mitigation measures). It is available to the public for free and is not proprietary.

In the guidance document, EPA provides six criteria for a model to qualify as a candidate for use in an attainment demonstration. These are listed and compliance with each is established in the following text.

- **The model has received a scientific peer review.** A formal scientific peer review of the UAM-V modeling system was conducted by ENSR (1993). Since that time, hundreds of scientists and modelers have reviewed the modeling system code as a routine part of their work with the modeling system.

- **The model can be demonstrated applicable to the problem on a theoretical basis.** As noted in the previous section, the UAM-V modeling system represents (either explicitly or implicitly) the physical and chemical processes that are currently known to influence the formation and transport of ozone as well as the emission, chemical transformation, and dispersion of ozone precursor pollutants. The features and capabilities of the modeling system are consistent with the application on a combined regional- and urban-scale, as required for this study.

- **Data bases needed to perform the analysis are available and adequate.** The UAM-V modeling system requires several different types of input data. These will be prepared using available data and EPA-recommended techniques. Their adequacy for use with the modeling system will be assessed as part of the modeling study.

- **Available past appropriate performance evaluations have shown the model is not biased toward underestimates.** Past applications of the UAM-V modeling system do not indicate a bias toward underestimation. Some examples of recent applications include OTAG (1997), BAAQMD (1998), the southeastern U.S. (Douglas et al., 1998), and the GCOS modeling study (Douglas et al., 2001). Each of these applications includes several days and day-to-day variations in model performance, but a consistent bias toward underestimation is not indicated.

- **A protocol on methods and procedures to be followed has been established.** The protocol is outlined in this document. The modeling will be conducted in a manner that is consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hour ozone standard.

- **The developer of the model must be willing to make the model available to users for free or for a reasonable cost, and the model cannot be proprietary.** Versions 1.24 and 1.3 of the UAM-V modeling system are available directly from SAI at no charge (see announcement on the EPA bulletin board to confirm this.) The UAM-V is not a proprietary model and as such complies with each element of the definition put forth recently by the North American Research Study of Tropospheric Ozone.

Applicability for Future PM Modeling

As noted earlier, the UAM-V modeling system is currently being upgraded to include aerosol chemistry. The aerosol component is designed to be more comprehensive and than that for both REMSAD and MODELS-3/CMAQ. The initial testing of UAMV-PM was completed in early 2003. A description of the new PM capabilities of UAM-V follows.

The UAM-VPM is based on the UAM-V, a three-dimensional Eulerian photochemical smog model that has been described elsewhere. The UAM-VPM differs from the UAM-V in that a fully integrated PM module is included. Simulation of particulate matter is considerably more difficult than gaseous species because particulates have both a size distribution (ca. 0.001- 70 μm radii particles) and a variable chemical composition. In addition, there are physical transformation processes, which occur uniquely for particulates. A detailed design document describing the mathematics behind each of the parameterizations is available from SAI. The approach taken for simulating each of the modeling platform features is outlined below:

1. **User Inputs and Dynamic Memory Allocation** - All PM specific input parameters and choices are passed to the model during initialization through user inputs. This includes the PM chemical species, the phases for those species, the equilibrium and irreversible PM chemical mechanisms, species-dependant PM physical constant data, and size resolution preferences. All system resources required by the model based on these

parameters are dynamically allocated during model initialization, and if insufficient resources are available, the user can re-examine the input options.

2. **Hybrid Sectional/Modal Size Distribution** - Detailed size resolution is required in specifying the size distribution function since many of the physical processes are size dependent. The classic methods are a sectional approach (adjacent, discrete size bins), and a modal approach (analytic functional form for the size distribution function). The modal approach uses few system resources and is good for lower-resolution calculations, whereas the sectional approach requires greater resources for higher resolution. We use a modal approach where high resolution is not necessary, and a sectional approach where it is, with algorithms for discretizing the modes into sections, and casting the sections back into modes. Any number of modes and sections can be used. This makes it possible to tailor the CPU resources required by the model to the hardware available, and yet still employ the state-of-the-science algorithms.

3. **Chemical Speciation** - PM species are calculated as pure modes ("externally mixed") for single compound emissions or unmixed fractions, and a single mixed mode ("internally mixed") for the result of any physical process that mixes different chemical species in the PM phase. Individual chemical species are assigned phases, which may be gas, inert liquid, aqueous, ionic, solid, or organic, and interactions between all these different phases are simulated. Both primary and secondary inorganic and organic species are simulated.

4. **Nucleation** - High concentration of gas phase sulfuric acid leads to formation of small particles. Theoretical parameterizations for nucleation at the present time do not reproduce data. Consequently, the relative humidity and temperature dependant parameterization of Fitzgerald and Hoppel (1998), which is based on experimental marine environment nucleation data, is used.

5. **Coagulation** - Coagulation is the process of two particles, of any size and composition, finding each other and combining to form a new particle. The process of finding each other can be due to Brownian motion, gravitational collection, turbulent inertial motion, or turbulent shear. The likelihood of combining and the effects of that combination are based on the parameterizations of Jacobson *et. al.* (1994) for combination of self-similar particles (homo-coagulation) and combination of dissimilar particles (hetero-coagulation). These algorithms preserve mass exactly.

6. **Growth** - Growth processes occur due to the interaction of existing particles with the gas phase. A particle may either grow or shrink due to such processes. The rates of growth or shrinkage depend on the relative humidity, the particle size, the particle composition (non-ideal Henry's law behavior due to high ionic strength) and the concentration fields. Particle ionic strength is calculated with an equilibrium chemistry solver. The parameterizations of Jacobson (1997) are implemented. These algorithms require little iteration, are unconditionally stable, and conserve mass exactly.

7. **Gas Phase Chemistry** - The UAM-V version 1.30 uses the Carbon Bond 99 (CB-99) chemical mechanism with updates to include the updated isoprene chemical mechanism

of Carter (1996), expanded treatment of toxics species, and improved representation of aldehyde photolysis. Additions to this mechanism to account for condensable secondary organic aerosol mass are based on the yield ratios of Pandis *et. al.* (1992) and later studies, but re-parameterized for the CB-99 mechanism.

8. **PM Equilibrium Chemistry** - Reversible reactions occur within particles, as well as between the gas phase and the particle phase. These include gas-to-particle mass transfer and visa versa, and ionization of solids or aqueous species in the PM phase, and visa versa. The species and reactions involved in equilibrium relations are input by the user, and are **not hardwired** into the model. Thus, the mechanism can easily be extended for research purposes, simplified to accommodate system constraints, or modified due to a particular concern for a specific application. An equilibrium chemistry solver, resembling the EQUISOLVE mass flux iteration methodology of Jacobson *et. al.* (1996) is employed, and water content is calculated with a Zdanovskii, Robinson and Stokes (ZSR) relationship (Jacobson, 1998).

9. **PM Irreversible Chemistry** - Irreversible chemistry occurs in the PM phase when there is significant water content in the PM phase (e.g. in the presence of clouds), and consists primarily of oxidation/reduction reactions which may or may not be catalyzed. Similarly to the equilibrium mechanism, the species and the mechanism are **not hardwired** into the code, but rather are read in during model initialization. This lends the same flexibility to the irreversible mechanism as is present in the equilibrium mechanism. An ordinary differential equation solver, similar to SMVGEAR, (Jacobson, 1995) will be employed. The first version of the model is a semi-dry version, appropriate for humid, but not wet conditions, and does not fully account for irreversible chemistry. Irreversible chemistry, coupled with extended treatment of toxics (primarily heavy metals) will be added in the next version.

10. **Model Inputs** - In additional to the usual UAM-V inputs (gas phase emissions, geographical files, and meteorological fields), the UAM-VPM requires a single user input file specifying the PM chemical mechanisms and species, and the necessary PM physical constants, as well as primary PM emissions inputs specifying species and size distributions and gridded in space and time. Default emissions options based on land-use characteristics are also available for testing purposes, and are application independent.

11. **Model Output** - In addition to the usual UAM-V model output files (simulated gas phase concentrations gridded in space and time), the UAM-VPM provides speciated PM size distribution functions, gridded in both space and time. These outputs are suitable for determination of simulated visibility detriments, simulated wet deposition, as well as health and other effects due to particulate matter.

The result is a scalable, portable, state-of-the-science, best-practice integrated photochemical ozone and PM modeling platform. Our plans for this modeling platform are to make it as widely available and as easy to use as is possible. To this end, it will be available on Unix class workstations, as well as high-end Windows NT PC machines. We would like to integrate it with a visualization and analysis environment for ease of use, and see it used as a training tool as well as a regulatory tool.

SELECTION AND OVERVIEW OF THE EMISSIONS MODELING AND PROCESSING TOOLS

The EPS2.5, BEIS-2, and MOBILE6 emissions processing/modeling tools have been identified for use in this study. EPS2.5 is an extended version of EPS (EPA, 1992) that has been enhanced to facilitate the preparation of regional-scale emission inventories. EPS2.5 was explicitly chosen for this study because it currently supports the detailed implementation of control measures that other available tools do not currently support. At this time, it is our assessment that EPS2.5 is the only tool that currently fully supports the features that are needed for representing the wide variety of emissions reduction measures that could be possibly considered for SIP modeling.

BEIS-2 is the latest available version of the EPA biogenic emission estimation model. Note that the UAM-V modeling system includes a representation of isoprene chemistry that is consistent with the use of BEIS-2.

MOBILE6.2 is the current version of the EPA tool for calculation of on-road motor vehicle emissions. However, since the modeling work for this attainment demonstration began before MOBILE6.2 was released (early 2001), the MOBILE6.0 model will be used for this attainment test. This is consistent with recent EPA guidance on the mobile model.

EPA (1999a) lists five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** EPS2.5 is designed for the preparation of detailed, regional- and urban-scale, modeling emissions inventories, as needed for this study. BEIS-2 is currently the recommended tool for estimation of biogenic emissions, which are likely to play an important role in ozone formation within the state of South Carolina. As noted earlier, MOBILE6.0 until recently was the operational version of the model developed and recommended by EPA for calculating emissions from on-road mobile sources. Use of this tool facilitates the use of the county-level estimates of vehicle miles traveled (VMT) and detailed temperature information available for this study.

- **Availability, documentation, and past performance should be satisfactory.** EPS2.5, BEIS-2, and MOBIEL6 are available for free and are fully documented. These tools have been used successfully in more than five recent applications including OTAG (1997), sub-regional modeling of the southeastern U.S. (Douglas et al., 1998) and the GCOS modeling analysis (Douglas et al., 2001).

- **Relevant experience of available staff and contractors should be consistent with choice of a model.** The modeling tasks will be performed by SAI staff members who are knowledgeable and experienced in the application of EPS2.5, BEIS-2, and

MOBILE6.0. SAI staff also attended a MOBILE6 workshop in January 2000. In addition transfer of the emissions processing/modeling tools and inventory databases as well as training/instruction in their use will position SC DHEC to refine and prepare additional modeling emissions inventories.

- **Time and resource constraints may be considered.** Use of EPS2.5, BEIS-2, and MOBILE6.0 is consistent with the proposed schedule and costs.

- **Consistency of the model with what was used in adjacent regional applications should be considered.** EPS2.5, BEIS-2, and MOBILE6 have recently been used for regional-scale modeling of the Atlanta, Birmingham, Baton Rouge, and GCOS areas. EPS2.5 was also used by the Minerals Management Service (MMS) for modeling of the effects of emissions from offshore oil and gas production on the Gulf Coast area. BEIS-2 was used for the OTAG regional-scale modeling effort.

Overview of EPS2.5

EPS2.5 is a series of FORTRAN modules that perform the intensive data manipulations required to incorporate spatial, temporal, and chemical resolution into an emission inventory used for photochemical modeling. It enables the user to conform to EPA emission inventory requirements, and evaluate proposed control measures for meeting required emission reductions. EPS2.5 provides emission inputs to the UAM-V and specific features and capabilities related to the UAM-V application are described later in this section.

Overview of BEIS-2

BEIS-2 is a computer algorithm used to generate emissions for air quality simulation models, such as UAM-V. Emission sources that are modeled include volatile organic compound (VOC) emissions from vegetation and nitric oxide (NO) emissions from soils. BEIS-2 includes an up-to-date, county-level biomass database and emission factors for a variety of plant species. It accommodates the use of solar-radiation information in calculating emission rates.

Overview of MOBILE6.0

The EPA's highway vehicle emission factor model, MOBILE6.0, is a FORTRAN program that provides average in-use fleet emission factors for volatile organic compounds (VOC), oxides of nitrogen (NO_x) and carbon monoxide (CO) for twenty-eight classes of vehicles, for any calendar year between 1970 and 2050 and under various conditions affecting in-use emission levels (e.g., ambient temperatures, average traffic speeds, gasoline volatility) as specified by the model user. It has been used in evaluating control strategies for highway mobile sources, by states (except California) and other local and regional planning agencies in the development of emission inventories and control strategies for SIPs, and in the development of environmental impact statements (EISs).

SELECTION AND OVERVIEW OF THE METEOROLOGICAL MODEL

The MM5 meteorological modeling system was selected for use in this study. MM5 is a state-of-the-science dynamic meteorological modeling system that has been used in several previous air quality modeling applications. Key features of the MM5 modeling system that are relevant to its use in this study include multiple nested-grid capabilities, incorporation of observed meteorological data using a four-dimensional data-assimilation technique, detailed treatment of the planetary boundary layer, and the ability to accurately simulate features with non-negligible vertical velocity components, such as the sea breeze and sub-grid-scale convection (a non-hydrostatic option). The MM5 modeling system is widely used and is currently supported by NCAR. Its use in conjunction with the UAM-V modeling system has been successfully demonstrated as part of a regional-scale modeling application for the southeastern U.S. (Douglas et al., 1998); its continued use for the GCOS and ATMOS studies has further enhanced our ability to successfully apply and use MM5 with UAM-V. This is achieved using the MM52UAMV software.

EPA (1999a) lists five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** The MM5 modeling system should enable a physically realistic simulation of the regional- and local airflow patterns, the sea-breeze, the boundary layer dynamics and other complex meteorological features that characterize South Carolina. The nested-grid feature will support the preparation of inputs for a regional-scale application of UAM-V.

- **Availability, documentation, and past performance should be satisfactory.** The MM5 modeling system is free and documentation is available. It has been used in conjunction with UAM-V to support regional-scale modeling of the southeastern U.S. and has been used for several other air quality modeling studies (e.g., California's San Joaquin Valley). It is currently being used for the GCOS and ATMOS modeling studies. Versions of the modeling system have been used for the past two decades to support research in the area of mesoscale meteorology.

- **Relevant experience of available staff and contractors should be consistent with choice of a model.** The modeling tasks will be performed by SAI staff members who are knowledgeable and experienced in the application of the MM5 modeling system and the coupling of the MM5 and UAM-V models. Recent, relevant experience includes application for the regional UAM-V modeling of Atlanta, Birmingham, and the eastern Gulf Coast area (Douglas et al, 1998), application for GCOS, preparation of MM5-derived meteorological inputs for UAM-V modeling of the western U.S. by EPA (Douglas et al., 1999a), 1-hour SIP modeling for Baton Rouge, and application for ATMOS. With the exception of the western U.S., each of these application included multiple nested grids with a 4 km high resolution grid. Through extensive testing and some simple modification of MM5, we have demonstrated considerable success in using MM5 for air quality modeling purposes.

- **Time and resource constraints may be considered.** Use of the MM5 modeling system is consistent with the proposed schedule and costs.

- **Consistency of the model with what was used in adjacent regional applications should be considered.** MM5 was recently used for regional-scale modeling of the southeastern U.S., with emphasis on Atlanta, Birmingham, and the eastern Gulf Coast. It is currently being used for GCOS and separately for additional regional-scale modeling of Louisiana. It is also being used for the ATMOS modeling study and for the penisular Florida ozone study. All of the modeling domains listed here include South Carolina.

Overview of MM5

A general description of this three-dimensional, prognostic meteorological model is found in Anthes and Warner (1978). The governing equations include the equations of motion, the continuity equations for mass and water vapor, and the thermodynamic equation. Those features relevant to this application are briefly described in this section.

The current version of MM5 can be applied in a non-hydrostatic mode for the improved simulation of small-scale vertical motions (such as those associated with the sea breeze and terrain effects). Use of this optional feature can be important to the accurate simulation of the airflow and other features at high horizontal resolution and will be utilized for this study.

The MM5 model employs the sigma vertical coordinate: $\sigma = (p - p_t)/(p_s - p_t)$, where p is pressure, p_t is the constant pressure specified as the top of the modeling domain, and p_s is the surface pressure. The sigma-coordinate surfaces follow the variable terrain. The governing equations are integrated over a grid that is staggered in the horizontal and vertical (Messinger and Arakawa, 1976). In the horizontal, the u and v wind components are calculated at points that are staggered with respect to those for all other variables. Along the vertical coordinate, vertical velocity is defined at the sigma levels while all other variables are defined at intermediate sigma levels.

The MM5 modeling system also supports the use of multiple nested grids. This feature is designed to enable the simulation of any important synoptic scale features at coarser resolution, while incorporating a high-resolution grid over the primary area(s) of interest. In this manner, the computational requirements associated with use of a high-resolution grid over a large domain are avoided. A one-way nesting procedure in which information from the simulation of each outer grid is used to provide boundary conditions for the inner grids is recommended.

To facilitate the realistic simulation of processes within the atmospheric boundary layer, variable surface parameters (including albedo, roughness length, and moisture availability) and a high-resolution planetary boundary layer (PBL) parameterization may be specified. The PBL parameterization also requires use of a multi-layer soil temperature model (an otherwise optional feature of MM5). For the coarse grids, several cumulus parameterization schemes are available to parameterize the effects of convection on the simulated environment. Several explicit moisture schemes are available for high-resolution grids.

The MM5 model supports four-dimensional data assimilation (FDDA), a procedure by which observed data are incorporated into the simulation. FDDA options include (1) "analysis nudging" in which the simulation variables are relaxed or "nudged" toward an objective analysis that incorporates the observed data and (2) "obs nudging" in which the variables are nudged toward individual observations.

The MM5 modeling system has been modified by SAI to include the output of the internally calculated vertical exchange coefficients (K_v) for use with UAM-V. This procedure for specifying K_v values based on MM5 simulation results was first implemented and tested by Douglas et al. (1998). Compared to the other options, this approach comes closest to representing the information that is required by UAM-V. Using this approach, the K_v values should reflect the effects of regional (for example, large-scale subsidence, sea breeze circulation systems, and possibly low-level jets), as well as local variables. Numerous studies have shown that these features can influence ozone concentrations.

Overview of the MM52UAMV Software

The MM52UAMV software, developed by SAI, maps the output from the MM5 model to the UAM-V grid(s). The MM5 output fields are first interpolated in the horizontal to the UAM-V grid. Typically, this entails (1) transformation from the map projection used by MM5 to that used by UAM-V and (2) interpolation to the UAM-V grid-cell center points. Interpolation is performed using a bi-linear scheme. If the grid resolution corresponding to the two projections is approximately equal, it is expected that features resolved by MM5 will also be present in the UAM-V ready fields.

The MM5 fields (as interpolated to the horizontal UAM-V grid) are then inverted (top to bottom) to accommodate the different vertical coordinate systems used by the two models and interpolated to the UAM-V layers using a linear interpolation scheme. All variables with the exception of the vertical exchange coefficients are interpolated to the grid-cell center heights. The vertical exchange coefficients are interpolated to the interface levels. Following interpolation, the meteorological variables are smoothed using a five-point algorithm. Optionally, the divergence present in the interpolated wind fields can be adjusted to limit or minimize the vertical velocity component at the top of the UAM-V modeling domain. If this option is invoked, the O'Brien vertical velocity adjustment procedure (O'Brien, 1970) is used to iteratively adjust the vertical velocity profile and horizontal wind fields such that the calculated divergence within each column of grid cells is less than a user-specified value. Finally, the meteorological variables are converted (as needed) to the units required by the UAM-V model and written out as UAM-V ready input files.

3 EPISODE SELECTION

The methods and results of the episode selection analysis to support the modeling exercise is described in this section. The analysis was performed by SC DHEC and major portions of this section were adapted from an SC DHEC internal report. This report is attached to the end of this protocol. For this first high-resolution photochemical model application for South Carolina, one episode was selected. This may be supplemented by additional episodes in the future.

Episode selection for the South Carolina modeling/analysis was based on a review of air quality data, and followed the methods described in the current (draft) EPA guidance (EPA, 1999). The years 1993, 1996, 1997, and 1998 were examined. For each year considered, design values were calculated using data for the current year, previous year, and following year. Quality assured ozone data for 1992 through 1999 were used.

The primary objective of the episode selection analysis was to identify suitable periods for analysis and modeling related to the 8-hour ozone NAAQS for the Anderson/Greenville/Spartanburg, Aiken/Columbia, Florence/Darlington, and Rock Hill areas in South Carolina. The approach to episode selection is consistent with current (draft) EPA guidance (EPA, 1999) on episode selection for 8-hour ozone attainment demonstration modeling. In this guidance, EPA lists the following as the most important criteria for choosing episodes:

- Monitored ozone concentrations comparable to the severity as implied by the form of the NAAQS
- Representation of a variety of meteorological conditions observed to correspond to monitored ozone concentrations of the severity implied by the form of the NAAQS
- Data availability
- Selection of a sufficient number of days so that the modeled attainment test is based on several days

EPA also provides several additional (secondary) criteria for episode selection:

- Episodes used in previous modeling exercises
- Episodes drawn from the period on which the current design value is based
- Observed concentrations are "close" to the design value for as many sites as possible
- Episodes are appropriate for as many of the nonattainment areas as possible (when several areas are being modeled simultaneously)

- Episodes that include weekend days

METHODOLOGY AND RESULTS

In accordance with EPA guidance, the primary objectives of the episode selection analysis were to identify candidate modeling episodes that

(1) represent the type of meteorological conditions that accompany ozone exceedances,

(2) are influenced by different airflow patterns (as primarily characterized by local wind speed and direction) on different days

(3) have ozone concentrations that are representative of the design value (the guidance quantifies the latter with a range of 10 ppb),

(4) have multiple days with maximum 8-hour ozone concentrations within 10 ppb of the design value for each site/area

(5) accommodate as many areas of the state as possible (with this initial modeling episode)[1].

Eight hour ozone data were examined for the years 1992 through 1999. The data were categorized according to ozone levels set forth in the (draft) EPA guidance. Eight-hour ozone values of 64 ppb or less were categorized as "low", those from 65 ppb to 84 ppb, as "moderate", 85 ppb to 105 ppb as "high", and greater than 105 ppb as "very high". The categorized data were then examined to determine the years for which the greatest number of high ozone values occurred. These totals along with information on ozone distributions relative to design values were the basis for the selection of years for which to further examine ozone data.

The frequency of occurrence of days within each of the ozone categories is presented in Table 3-1. (The lowest category has been dropped from the table.)

TABLE 3-1a. Summary of maximum 8-hour ozone concentrations for South Carolina for 1992-1999

Year	Moderate	High	Very High
	65 ppb ≤ O_3 < 85 ppb	85 ppb ≤ O_3 < 105 ppb	≥105 ppb
1992	113	6	0
1993	827	64	7
1994	387	43	0

[1] This is an important consideration for this study, since this is the first detailed photochemical modeling exercise for South Carolina. This modeling exercise will therefore facilitate the evaluation of the emissions inventory and the ability of the modeling system to simulate ozone concentration levels and patterns both regionally and in different parts of the State.

1995	568	45	2
1996	139	3	0
1997	861	65	0
1998	1089	190	8
1999	1072	149	5

The totals for the High and Very High categories represent the number of exceedances of the 8-hour standard for all of South Carolina for each year. There is a peak in the number of exceedances in 1993 and then again toward the end of the period. If the newly proposed 8-hour standard was in effect in 1993, South Carolina would have recorded 71 exceedances. Seven of those would have fallen in the "Very High" category. Lower ozone levels were recorded in 1992, 1994, 1995, and 1996. Based on the proposed 8 hour standard, only three exceedances would have occurred statewide during 1996. The greatest number of exceedances, 198, occurred in 1998.

To represent years in which a low number and high number of exceedances occurred, the years of 1993, 1996, 1997, and 1998 were analyzed. Although episode selection was carried out for all four years; the results for 1998 are presented here. Because the ozone season of 1998 was the worst on record, the analysis yielded a potentially rich data set for ozone modeling – and potentially several episodes that are representative of current design values.

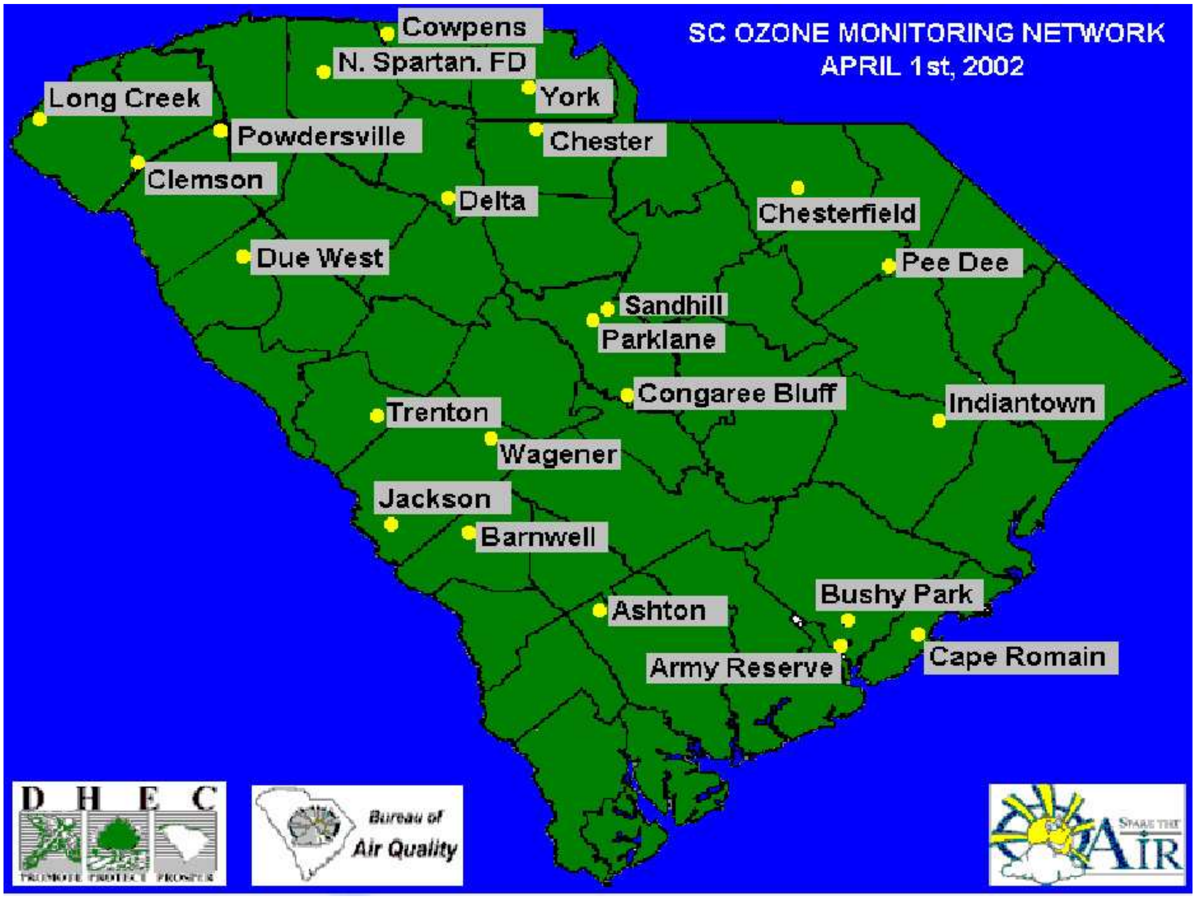
The selection of the ozone episode for 1998 was a multi step process. In the first step, design values were calculated for each monitor in South Carolina for 1998. The design values for 1998 are calculated by averaging the 4th highest ozone value for each monitor from 1997, 1998, and 1999. If the design value of any monitor were less than 75 ppb, (10 ppb below the standard) the monitor was excluded from the analysis. All monitors had design values greater than 75 ppb. Design values for 1997-1999 are presented in Table 3-2.

Table 3-2. 1997-1999 design values for South Carolina monitoring sites used for 75 ppb screening test.

Monitor	County	1997-1999 Design Value	Monitor	County	1997-1999 Design Value
Cape Romain	Charleston	79	Chester	Chester	91
Army Reserve	Charleston	75	Clemson	Pickens	90
Bushy Park	Berkeley	79	Cowpens	Cherokee	93
Indiantown	Williamsburg	75	Due West	Abbeville	86
Sand Hill	Richland	90	Long Creek	Oconee	86
Congaree Swamp	Richland	75	North SPA	Spartanburg	94
Pee Dee	Darlington	88	Powdersville	Anderson	95
Parklane	Richland		York	York	

		92			86
Trenton	Edgefield	85	Ashton	Colleton	82
Jackson	Aiken	89	Delta	Union	84
			Barnwell	Barnwell	88

Fig. 3-1 SC Ozone Monitoring Network



In the second step and third steps, the top 8-hour ozone concentrations for each of the three years (1997 – 1999) were listed and then averaged. In the fourth step, all 8-hour average ozone concentrations within 10 ppb of the fourth average high at each monitor were identified. Table 3-3 shows the range of values noted at each monitor. It is in this step, that ozone values and dates (based on the ozone concentrations within the given range) were selected for modeling purposes. Once these dates were selected, then they were classified by meteorological conditions with emphases on the wind parameters.

Table 3-3. Range of values within 10 ppb of the 4th highest 8-hour ozone concentration at each site.

Monitor	**AIRS ID No.**	**Range**	**Monitor**	**AIRS ID No.**	**Range**
Cape Romain	45-019-0046-1	70 - 90	Clemson	45-077-0002-1	82 – 102

Army Reserve	45-019-0042-1	66 – 86	Cowpens	45-021-0002-1	83 – 103
Bushy Park	45-015-0002-1	69 – 89	Long Creek	45-073-0001-1	83 – 103
Jackson	45-003-0003-2	79 – 99	N. Spartanburg	45-083-0009-1	86 – 106
Barnwell	45-007-0003-1	78 – 98	Powdersville	45-007-0003-1	86 - 106
Congaree	45-079-1006-2	66 – 86	Pee Dee	45-031-0003-1	80 – 100
Sand Hill	45-079-1002-1	81 – 101	York	45-091-0006-1	77 - 97
Parklane	45-079-0007-1	83 – 103	Ashton	45-029-0002-2	73 - 93
Chester	45-023-0002-1	83 - 103	Delta	45-087-0001-1	75 - 95
			Indiantown	45-089-0001-2	69 - 89

Seven ozone episodes were selected and examined for the 1998 season. The episode for the period 15 - 22 May is presented here. Based on the EPA ozone selection procedure, dates in bold italics in Table 3-4 represent days in which the maximum 8-hour average ozone levels were within 10 parts per billion of the design values for a given monitor. The Table divides South Carolina into four regions (Coastal, Midlands, Upstate, and Central Savannah River Area or CSRA). This helps to identify the regional impact of the ozone episode. Note that all areas were impacted by this early season event. During this period, a stagnant, flat upper-ridge was centered over the Gulf of Mexico, and extended northward into the Deep South and Southeast. This position of the upper-high cut off the moisture from the Gulf of Mexico, and resulted in unseasonably hot and dry weather in South Carolina.

The final step in the selection of ozone episodes was to classify the days from Table 3-4 by wind speed and direction. Table 3-5 lists examples of classification for several monitors during this May episode. On 16 May, the maximum 8-hour average ozone concentration at Army Reserve was within 10 ppb of the standard with a wind speed of 5 mph from the south-southwest. On 18 May, the average was with 10 ppb of the design value and exceeded the 8-hour ozone standard, but the winds were from the east-southeast at 7.9 mph. These data yield a variety of different wind directions and wind speeds, thus satisfying the EPA guidance.

Examination of the total percent (over all monitors) a given day had ozone levels within 10 ppb of the design value at a particular monitor (Table 3-4), resulted in the selection of 18 – 22 May for future air quality modeling. A cut-off of 50 percent, with respect to the number of days that meet the 10 ppb criteria, was used to distinguish the key days and define the episode period. On these days, 67, 81, 67, 62, and 52 percent of the monitors respectively, recorded 8-hour ozone concentrations within 10 ppb of the monitor design value.

TABLE 3-4. Episode days with 8-hour ozone values within 10 ppb of the design value at a given monitor (bold italics). Percentages (shaded) represent number of monitors for region meeting criteria for given day.

Monitor	Date							
Cape Romain	15-May	**16-May**	17-May	18-May	19-May	20-May	21-May	22-May
Army Reserve	15-May	***16-May***	***17-May***	***18-May***	***19-May***	***20-May***	***21-May***	***22-May***
Ashton	***15-May***	***16-May***	17-May	***18-May***	***19-May***	***20-May***	***21-May***	***22-May***
Bushy	15-May	***16-May***	17-May	***18-May***	***19-May***	***20-May***	***21-May***	***22-May***
Indian	***15-May***	***16-May***	17-May	***18-May***	19-May	***20-May***	***21-May***	***22-May***

Coastal %	40%	80%	20%	80%	60%	80%	80%	C80%
Sandhill	***15-May***	***16-May***	17-May	18-May	***19-May***	***20-May***	***21-May***	22-May
Parklane	***15-May***	16-May	17-May	18-May	***19-May***	***20-May***	21-May	22-May
Congaree	15-May	16-May	17-May	18-May	***19-May***	***20-May***	***21-May***	***22-May***
Pee Dee	15-May	***16-May***	17-May	***18-May***	***19-May***	20-May	***21-May***	22-May
Midlands %	50%	50%	0%	25%	100%	75%	75%	25%
Chester	***15-May***	16-May	17-May	***18-May***	***19-May***	***20-May***	***21-May***	22-May
Clemson	15-May	16-May	17-May	***18-May***	***19-May***	20-May	21-May	***22-May***
Cowpens	***15-May***	16-May	17-May	***18-May***	***19-May***	***20-May***	21-May	22-May
Delta	15-May	16-May	17-May	***18-May***	***19-May***	***20-May***	***21-May***	22-May
Due West	15-May	16-May	17-May	***18-May***	***19-May***	***20-May***	***21-May***	***22-May***
Longcreek	15-May	16-May	17-May	18-May	***19-May***	20-May	21-May	22-May
N Spartanburg	***15-May***	16-May	17-May	***18-May***	***19-May***	***20-May***	21-May	22-May
Powdersville	15-May	16-May	17-May	***18-May***	19-May	20-May	21-May	***22-May***
York	15-May	16-May	17-May	***18-May***	***19-May***	***20-May***	***21-May***	22-May
Upstate %	*33%*	*0%*	*0%*	*88%*	*88%*	*67%*	*44%*	*33%*
Barnwell	***15-May***	16-May	17-May	***18-May***	***19-May***	20-May	***21-May***	***22-May***
Jackson	15-May	16-May	17-May	18-May	19-May	***20-May***	***21-May***	***22-May***
Trenton	15-May	16-May	17-May	18-May	***19-May***	20-May	21-May	***22-May***
CSRA%	33%	0%	0%	33%	67%	33%	67%	100%
Total %	38%	29%	5%	**67%**	**81%**	**67%**	**62%**	**52%**

TABLE 3-5. Wind speed (Ws) and wind direction (Wd) for selected monitoring sites for key days of the May 1998 episode period.

Ashton	Ws	Wd	Bushy Park	Ws	Wd
5/18/98	7.9	70	5/18/98	7.9	70
5/19/98	5.5	120	5/19/98	5.5	10
5/20/98			5/20/98	9.1	240

As indicated in Table 3-4, the days listed in Table 3-5 are key days with ozone concentrations within 10 ppb of the site-specific design value.

FINDINGS FROM A RELATED STUDY

Results from a recent episode selection analysis designed to identify historical ozone episode periods suitable for use in conducting analysis and modeling activities related to 1-hour and 8-hour ozone for (potential) nonattainment areas in the northern portions of Georgia and Alabama (Douglas et al., 1999b) were examined to see if these days were also picked up using a different approach for neighboring areas. The methodology used for this other episode selection analysis was based on that developed for the Southern Appalachian Mountains Initiative (SAMI) episode selection study by Deuel and Douglas (1998). Days within the analysis period (1990-1998) were classified according to meteorological and air quality parameters using the Classification and Regression Tree (CART) analysis technique. The frequency of occurrence of ozone exceedances for each classification type was then determined for each of the areas of interest. Days with maximum ozone concentrations within approximately 10 ppb of the respective design values were also identified. Finally, an optimization procedure was applied to the selection of multi-day episodes for maximum achievement of the specified episode selection criteria (as outlined above) for various combinations of geographical areas and ozone metrics (i.e., 1-hour and 8-hour ozone).

Results for the Atlanta area do not indicate that these episode days represent typical meteorological/ozone exceedance regimes for the Atlanta. However, 8-hour ozone concentrations greater than 100 ppb were recorded at one or more of the Atlanta-area monitoring sites on all five days, with a maximum 8-hour value of 125 ppb on 19 May.

Results for the Augusta, Georgia area (located along the Georgia/South Carolina border) were also examined. Of the five May 1998 South Carolina episode days, three days, 19-21 May, were classified as representative of frequently occurring meteorological/ozone exceedance regimes. Maximum 8-hour ozone concentrations greater than 85 ppb were recorded on four of the five days (19-22 May), with a maximum 8-hour value of 105 ppb on 20 May.

The finding for Augusta (from this alternative episode selection analysis) indicate that period 18 – 22 May is valid for modeling purposes. The data for Augusta and Atlanta suggest that this was a regional event and that there is some potential for regional-scale transport.

OTHER CONSIDERATIONS

A typical modeling episode periods includes 2 to 3 start-up days (during which the influence of the initial conditions, which are not well known, is expected to be greatest) and one clean out day (used for model evaluation purposes to ensure that the model is able to simulate both higher and lower ozone concentration days). It is also desirable to initiate the simulation when the ozone concentrations are relatively low, so that day-to-day carryover (of ozone) from the start-up days to the primary days is minimized (this is important if the concentrations for the start-up days are not accurately simulated).

Based on a review of the ozone data for sites in South Carolina (as well as Atlanta and Augusta), the recommended modeling period is 16-23 May. This eight-day period begins and ends on a Saturday. Thus all key modeling days are weekdays.

SUMMARY

In summary, it appears that the 16 – 23 May 1998 period provides a good basis for modeling for all four areas from the perspective of capturing multiple high ozone days and some different wind directions for the South Carolina monitoring sites. The key modeling days are 18-22 May. The episode provides a good first episode for modeling because several different areas of the state are affected, thus allowing an evaluation of the emissions inventory as well as the ability of the modeling system to replicate the observed ozone concentrations patterns and levels. The results of the methodology used for this analysis was backed by results from a related study done for the Augusta area in neighboring Georgia.

4 PHOTOCHEMICAL AND METEOROLOGICAL MODELING DOMAIN SPECIFICATION

The modeling domain for application of the UAM-V was designed to accommodate both regional and subregional influences as well as to provide a detailed representation of the emissions, meteorological fields, and ozone (and precursor) concentration patterns over the area of interest. The UAM-V modeling domain is presented in Figure 4-1 and includes a 36-km resolution outer grid encompassing the southeastern U.S; a 12-km resolution intermediate grid; and a 4-km resolution inner grid encompassing South Carolina and portions of Georgia, Tennessee, and North Carolina.

The regional extent of the modeling domain is intended to provide realistic boundary conditions for the primary area of interest and thus avoid some of the uncertainty introduced in the modeling results through the incomplete and sometimes arbitrary specification of boundary conditions. The offshore extent of the domain is designed to accommodate the simulation of over-water pollutant transport and recirculation. The use of 4-km grid resolution over the entire State of South Carolina is consistent with an urban-scale analysis of all of the areas of interest.

The UAM-V domain is further defined by eleven vertical layers with layer interfaces at 50, 100, 200, 350, 500, 750, 1000, 1250, 1750, 2500, and 3500 meters (m) above ground level (agl). Further testing of the appropriateness of the vertical grid structure may be performed as part of the diagnostic testing, as described in Section 7 of this protocol document.

The modeling domain for application of MM5 is shown in Figure 4-2. This domain is much larger than that for UAM-V, in order to enable the simulation of any important synoptic scale features and their influence on the regional meteorology. The modeling domain consists of an extended outer grid with approximately 108-km horizontal resolution and four inner (nested) grids with approximately 36, 12, and 4-km resolution. The horizontal resolution was specified to match that for UAM-V. A one-way nesting procedure and 22 vertical levels will be employed. The vertical grid is defined using the MM5 sigma-based vertical coordinate system. The layer thickness increases with height such that high resolution is achieved within the planetary boundary layer. The vertical layer heights for application of MM5 are listed in Table 4-1.

TABLE 4-1. MM5 vertical levels for the SC DHEC application.

Level	Sigma	Average Height[2] (m)
1	0.996	30
2	0.988	80
3	0.982	125
4	0.972	215
5	0.960	305
6	0.944	430
7	0.928	560
8	0.910	700
9	0.890	865
10	0.860	1115
11	0.830	1370
12	0.790	1720
13	0.745	2130
14	0.690	2660
15	0.620	3375
16	0.540	4260
17	0.460	5240
18	0.380	6225
19	0.300	7585
20	0.220	9035
21	0.140	10790
22	0.050	13355

[2] Approximate heights – to be updated following initial application of MM5.

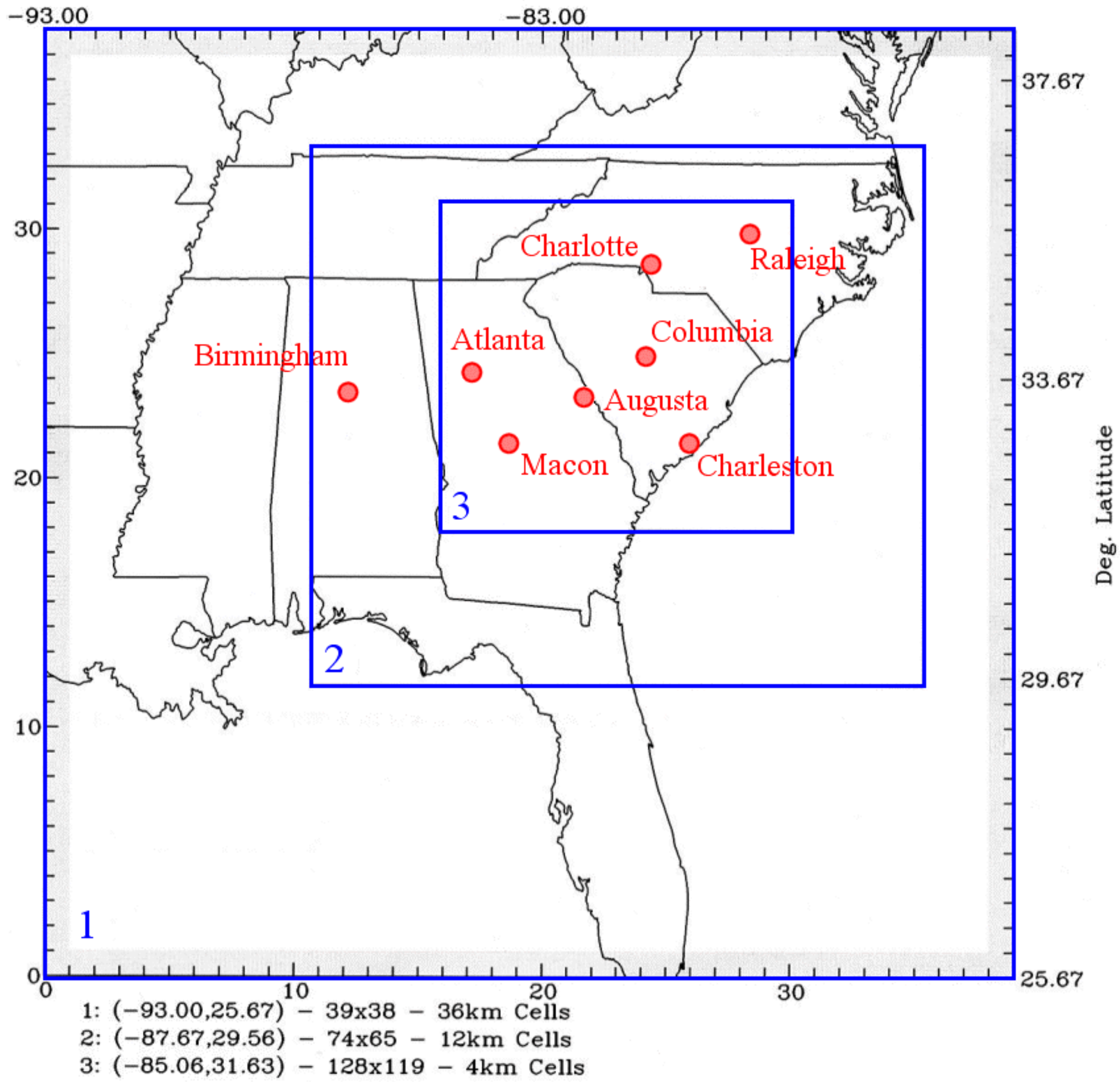


FIGURE 4-1. UAM-V modeling domain for the South Carolina 8-hour ozone modeling study.

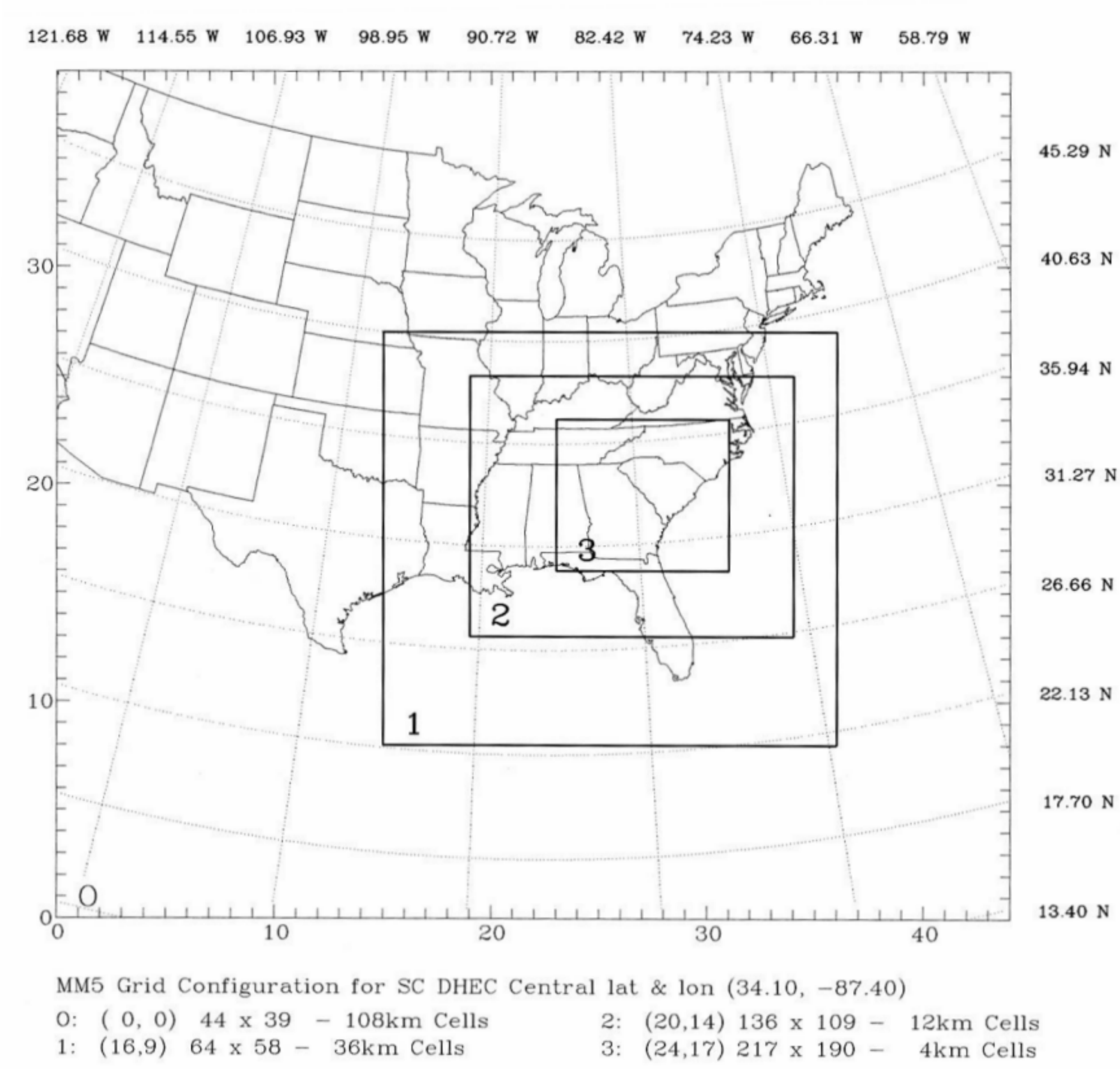


FIGURE 4-2. MM5 modeling domain for the South Carolina application.

5 INPUT PREPARATION

Version 1.30 of the UAM-V modeling system will be used for the South Carolina modeling analysis. This latest version of the model accommodates the use of a variety of horizontal coordinate systems and either the standard or enhanced ("fast") chemistry solver. It also includes process analysis capabilities.

The UAM-V modeling system requires a variety of input files that contain information pertaining to the modeling domain and simulation period. These include gridded, day-specific emissions estimates and meteorological fields; initial and boundary conditions; land-use information; and chemistry parameters. The methods and data to be used in preparing the UAM-V inputs for the base-case modeling exercises are described in this section of the protocol document.

BASE-YEAR EMISSION INVENTORY PREPARATION

The UAM-V requires specification of gridded low-level emissions for the full domain and each subdomain. Elevated point source emissions for all sources within the domain are contained in a single input file. The preparation of these input files is described in this section. The procedures presented here are consistent with EPA guidance on the preparation of emissions inventories for ozone, particulate matter, and regional haze (EPA, 1999b).

Emission Inventory Requirements for Modeling: Background and Objectives

In order for photochemical simulation models to accurately predict temporal and spatial variations in modeled ozone concentrations, the emission inventories input to these models must contain considerably more detail than an inventory generated to meet periodic emission inventory reporting requirements. The primary additional requirements of the photochemical modeling inventory are summarized below. This information is primarily derived from the EPA guidance document entitled *Procedures for the Preparation of Emission Inventories for Carbon Monoxide and Precursors of Ozone, Volume II: Emission Inventory Requirements for Photochemical Air Quality Simulation Models*, prepared for EPA by SAI in 1992.

Spatial Allocation: Emission estimates of precursor pollutants must be provided for each individual cell of a grid system within the modeling domain instead of at a county or regional level.

Temporal Allocation: Emissions must be specified as hourly rather than annual or daily rates. Additionally, annual or seasonal average rates should be adjusted to reflect episodic or day-specific conditions as accurately as possible.

Chemical Speciation: Total reactive VOC and NO_x emissions estimates must be disaggregated into several classes of VOC and NO and NO_2, respectively; spatially and temporally resolved emission estimates of CO are also required.

Stack Parameters: For models such as the UAM-V that provide for vertical resolution of pollutants, stack and exhaust gas parameters must be provided for each large point source.

Each of these is discussed further below.

Spatial Allocation of Emissions

Point Sources. Point source locations are typically reported to within a fraction of a kilometer; assigning emissions from these sources to the appropriate grid cell is simple.

Area Sources. By contrast, spatial resolution of area source emissions requires substantially more effort. Two basic methods can be used to apportion area source emissions to grid cells. The most accurate (and resource-intensive) approach is to obtain area source activity level information directly for each grid cell. The alternative approach, more commonly employed, is to apportion the county-level emissions from the existing annual inventory to grid cells using representative apportioning factors for each source type.

This latter approach requires the determination of apportioning factors based on the distribution of some spatial surrogate indicator of emission levels or activity (e.g., population, census tract data, or type of land use) for each grid cell. These factors are then applied to the county- or parish-level emissions to yield estimates of emissions from that source category by grid cell. The major assumption underlying this method is that emissions from each area source category behave spatially in the same manner as the spatial surrogate indicator. In most large urban areas, local planning agencies can provide detailed land use, population, or in some cases, employment statistics at the subcounty level. These data can be used to spatially apportion most of the area source emissions in the modeling inventory.

A spatial surrogate indicator is a parameter whose distribution is known at a sub-county level and which behaves similarly to the activity levels of interest. Commonly used spatial surrogate indicators include land-use parameters, employment in various industrial and commercial sectors, population, and dwelling units. Different surrogate indicators can be used to apportion emissions for the various area source categories, of course, depending on which of the available indicators best describes the spatial distribution of the emissions.

Mobile Sources. Planning, land-use, and transportation models are already in use in many urban areas, and can provide much of the data necessary to allocate mobile source emissions and develop emission estimates by link for highway motor vehicles. Such models are also generally capable of developing forecasts for future years which can be utilized in the development of projection inventories.

Mobile sources differ from stationary source categories in that their spatial variation is more accurately described using a link-based rather than a surrogate-based gridding procedure. In a link-based spatial allocation approach, emissions are distributed only to those grid cells that contain transportation pathways (e.g., roadways, railways, airports, shipping channels, etc.). This approach is usually used in conjunction with a surrogate-based procedure to complete the spatial resolution of the mobile source inventory.

Emissions from on-road vehicles on limited access roadways (interstates and expressways), railroad locomotives, aircraft, and vessels are often spatially allocated with a link-based procedure, since the transport routes used by these vehicles are both identifiable and readily modeled as a series of lines or links. This results in more accurate allocation of emissions from these sources than could be achieved using surrogates such as population or land use.

Non-link surrogates are commonly used to spatially allocate mobile emissions in the following situations:

- Links are too numerous to define and process, as is typically the case for on-road rural and urban vehicles and for off-road vehicles.

- Emission totals are too insignificant when compared with emissions from other sources in the modeling domain to warrant the development of link data.

- Use of gridded spatial surrogates based on land-use or population data provides a more accurate allocation of vehicle emissions. For example, recreational boating activities may be distributed approximately equally over the surface of a large lake.

In most modeling applications, a combination of link and land-use surrogates is used for the spatial allocation of mobile source emissions.

Temporal Resolution of Emissions

In order to simulate hourly concentrations of ozone and other pollutants, photochemical models require hour-by-hour estimates of emissions at the grid cell level. Several approaches can be used to provide the temporal detail needed in the modeling inventory. The most accurate and exacting approach is to determine the emissions (or activity levels) for specific sources for each hour of a typical day in the time period being modeled.

As an alternative, typical hourly patterns of activity levels can be developed for each source category. These are then applied to the annual or seasonally adjusted emissions to estimate hourly emissions. This approach is commonly employed for area sources, including highway motor vehicles, and is usually used for all but the largest point sources.

Usually, the photochemical air quality model is applied for an episode in the season of the year in which meteorological conditions are most conducive to ozone formation; for most locations, this means the summer months (i.e., May through September). By contrast, CO non-attainment episodes often occur in the winter months. Consequently, emissions must be adjusted to reflect typical levels for the particular non-attainment season (ozone or CO).

Similarly, emissions are usually adjusted to represent the day of the week on which polluting activities are at a maximum, normally a weekday. In some cases (such as validation studies), simulating weekend conditions when automotive and industrial emission levels are different may be useful. For this purpose, additional temporal pattern information pertaining to weekend days must be used to construct a weekend modeling inventory. In many urban regions, the second may not be possible for highway vehicles, since transportation models may only be based on information (e.g., travel pattern surveys) applicable only for weekday situations. If the model is to be used to estimate ambient concentrations of various pollutants for time periods other than the ozone season, additional seasonal information may be required.

Point Sources. The modeling inventory should represent as accurately as possible day-specific emission estimates for each hour of the modeling episode. By contrast, the existing point source inventory will more likely contain annual or typical ozone season day estimates of emissions and a general description of the operating schedule (seasonal fractions of annual throughput, and operating schedule in terms of weeks/year, days/week, and hours/day in operation).

Ideally, each facility would be contacted to obtain hourly operating records for the modeling episode, or, if this information is unavailable, representative operating schedules for a typical ozone season day. Certain local agencies may also have this type of temporal information. Some sources for which this type of data may be available include the following: power plants (which generally keep detailed, hourly records of fuel firing rates and power output for each day of operation), major industrial facilities such as automotive assembly plants and refineries, and tank farms.

For many smaller point sources, reasonable temporal resolution can be obtained from the operating data that are typically collected for each point source.

Area Sources. Since the basic area source inventory usually contains estimates of annual (or sometimes seasonally adjusted) emissions, the emissions modeler must expend additional effort to estimate hour-by-hour emission rates for the episode days. Several approaches can be employed to develop hourly emissions resolution; all involve the use of assumed diurnal patterns of activity. In addition to hourly patterns, estimates of seasonal fractions of annual activity will be needed if the county-level inventory is not seasonally adjusted. Activity profiles by day of week will also be required.

Mobile Sources. Temporal adjustment of the mobile source inventory into monthly, daily, and hourly specific totals is not significantly different than the treatment of other area source categories. If hourly vehicular speeds and VMT distributions are available from the local Metropolitan Planning Organizations (MPOs), these can be utilized in estimating hourly mobile source emissions.

Chemical Resolution of Emissions

Because photochemical models like the UAM-V are intended to simulate actual photochemistry, they utilize different chemical reactions for various types of VOCs and require specific information as to the proportions of these various types present in the inventory. For this reason, VOC emission totals must be disaggregated into subtotals for various chemical classes. NO_x emissions also have to be distributed as NO and NO_2.

Literally thousands of individual chemical compounds typically compose the total VOC emissions in an urban area. No photochemical model considers each organic compound individually; instead, VOC emissions are distributed into chemical classes which behave similarly in photochemical reactions. The UAM-V employs a carbon bond classification scheme based on the presence of certain types of carbon bonds in each VOC molecule.

Two basic approaches can be followed for determining split factors. Ideally, VOC split factors should be source-specific, reflecting the actual composition of VOC emissions. In some instances, source-specific VOC species data may be available for certain individual facilities (perhaps through source tests or material composition considerations). Generally, however, most industries cannot provide reliable VOC or NO_x species data or accurately apportion their emissions into appropriate classes, in which case generalized VOC and NO_x distributions must be assumed for various source categories.

Because of resource limitations and unavailability of solvent composition data, however, collecting source-specific speciation data is generally impractical for all but a very few large point or area source emitters. An alternative method employs generalized VOC speciation data from the literature to develop VOC split factors by source type.

<u>Elevated Point Source Requirements</u>

The UAM-V assigns emissions from point sources to elevated grid cells if they are characterized by an effective stack height (i.e., the sum of the physical height of the stack and any plume rise) that is greater than the height of the grid cell. Accordingly, the emission inventory must include stack information (e.g., physical stack height and diameter, stack gas velocity, and temperature) for the major point sources in the area.

The objective of the emissions preparation task is to prepare high quality modeling emission inventories for use in the photochemical model application, making use of available data and appropriate gridding, temporal allocation, and speciation techniques.

Acquisition of Emissions Data

A first and important step in the emissions processing task is the acquisition of data for preparation of the inventories. From the starting point of the data and information that SAI has obtained as part of the GCOS and ATMOS modeling analyses we will identify and collect additional data for use in this study. We propose to base the modeling inventory primarily on EPA's 1996 National Emissions Trends (NET) inventory (Version 3). To ensure the most accurate estimation of base-year ozone precursor emissions for the modeling, we will also obtain the latest information available for South Carolina, North Carolina, Georgia, and Florida (if this is different from what we already have in-house for the GCOS and ATMOS modeling studies) and incorporate these data into the modeling inventory. Specifically, we will request the following from the State, local agencies, MPO's and industrial participants (as appropriate):

- Area source data (county/parish level emission estimates, population, and activity)

- Point source data (stack parameters, emission rates, etc.)

- Mobile sources data (VMT, speeds, fleet mix, fuel characteristics, program characteristics, etc., and/or transportation model output, including network configuration)

- Supporting information (if any) needed to adjust the emission estimates to the levels required for the episodic and future simulation year levels (e.g., demographic or economic growth between the inventory year, the base-year, and the future years (2007 and 2012))

In addition to the emissions data described above, we will also obtain information, as available, that will permit the appropriate spatial, temporal, and chemical resolution of the inventory. These data may take the form of:

- Gridded demographic, economic, or land-use data that can be used to spatially allocate area source emissions (typically, these are represented as the fraction of the total activity for each indicator within a county that is located within a given grid cell)

- Link-based activity data (or emissions) for mobile sources

- Region-specific and/or year-specific temporal profiles for area source categories

- Source-specific operating data (hours per day, days per week, weeks per year, monthly or seasonal fractions of annual throughput)

- Region- or source-specific chemical speciation data

Obviously, not all of this information will be available for each source or source category in the inventory. Attention will be focused on acquiring the best available data for the largest sources within a given area.

Episode-Specific Information

To further refine the base-year inventories, it is desirable to refine the annual inventory to incorporate known differences for the specific episode being simulated. For example, if a particular large point source (for example, a SCE&G unit) was not operating during the episode, this information should be incorporated in the episode-specific inventory. Emission estimates should also be adjusted to reflect seasonal conditions. We will thus obtain any available episode-specific and/or seasonal information that would affect any portions of the inventory for the episode.

For each episode to be modeled, the types of information needed include the following:

- Daily (or preferably hourly, if available) emissions data for major point sources for each of the episode days. If significant differences in associated stack parameters such as temperature, flow rate, and velocity are documented, these data can be used as well.

- List of sources not in operation for each episode day.

Our experience in working with SCE&G, Santee Cooper, CP&L, Duke Energy, and Southern Company will facilitate our ability to collect and incorporate episode specific information from these important sources.

Emissions Processing Tools and Procedures

Preparation of the modeling inventories involves many steps. To facilitate development of the detailed emission inventories required for photochemical modeling for this analysis, a version of the EPA UAM Emissions Preprocessor System (EPS 2.5) will be used.[3] This system, originally developed by SAI under the sponsorship of the EPA's Office of Air Quality Planning and Standards, consists of a series of computer programs designed to perform the intensive data manipulations necessary to adapt a county-level annual or seasonal emission inventory for modeling use. EPS 2.5 provides the capabilities to support the CAAA requirements, to conform to EPA emission inventory requirements, and to allow the evaluation of proposed control measures for meeting Reasonable Further Progress (RFP) regulations and special study concerns.

<u>Application of EPS2.5, BEIS, and MOBILE</u>

The core EPS 2.5 system consists of a series of FORTRAN modules that incorporate spatial, temporal, and chemical resolution into an emissions inventory used for photochemical modeling. EPS 2.5 system input files which must be created specific to each modeling region include: (1) projection factors used to forecast or backcast emission rates from the year of input emissions to the episode modeling year, (2) gridded area, population, and land use surrogates used to spatially allocate area source emissions, and (3) digitized link data used to spatially allocate selected source categories (routinely mobile sources). Point, area, and mobile source emission data are usually processed separately through the EPS 2.5 system to facilitate both data tracking for quality control and the use of the data in evaluating the effects of alternative proposed control strategies on predicted air pollutant concentrations.

Point source data will be initially processed by the PREPNT module, which performs an initial screening of the data to determine whether each source will be treated as low-level or elevated. PREPNT also converts the input data to the EPS 2.5 internal Emission Model Binary Record (EMBR) format. The point source inventory is then ready for projection to future year levels, temporal allocation, and chemical speciation.

County-level (or other aggregated) area and mobile source emissions data enter the EPS 2.5 system through the PREAM module, which separates the area and on-road motor vehicle emissions data into two files. (If data for calculating link-based mobile source emissions are available, the LBASE module serves as the entry point for these data.) The emissions files created by PREAM are in the EMBR format. The PREAM module also disaggregates total motor vehicle emissions, which are usually reported in the input data by road type (limited access, urban, suburban, and rural) and vehicle class (light-duty gasoline vehicles,

---

[3] For biogenic emissions, the latest available version of EPA's Biogenic Emissions Inventory System (BEIS) will be used. Currently, this is BEIS2, but BEIS3 may be released in time for use in this study.

light-duty gasoline trucks, heavy-duty gasoline vehicle, and heavy-duty diesel vehicle), into the four emission component categories employed by EPA's MOBILE models (versions 4.0 and higher): exhaust, evaporative, refueling losses, and running losses. The on-road motor vehicle emissions will be adjusted to reflect episodic and scenario-specific conditions, such as existing or proposed Inspection and Maintenance (I/M) programs, Stage II vapor recovery controls, and ambient temperatures. We will follow the traditional approach of using major highway networks and population data, along with county-level VMT to estimate and spatially allocate emissions to the appropriate grids.

Each of the inventory components (e.g., point sources, area sources, on-road motor vehicles) will then be processed separately through the remaining modules of EPS 2.5 to facilitate quality control tracking and control strategy analysis. After projection to the year to be modeled (performed by the CNTLEM module), each file will be chemically speciated and temporally allocated by the CHMSPL and TMPRL modules, respectively. For area sources, non-road mobile sources, and on-road motor vehicles, county-level emission totals by source category will be spatially allocated to individual grid cells in the UAM-V modeling domain by the GRDEM module; point source emissions will be allocated to grid cells based on source location. Day-specific biogenic emissions will be prepared using BEIS-2 and the MM5-derived temperature and solar radiation fields. The gridded anthropogenic emissions files will then be merged with the biogenic emissions file into a single low-level emissions file, as the final step prior to input to the UAM-V.

Selection of Sources for P-i-G Treatment

Point sources for plume-in-grid (P-i-G) treatment will be selected according to NO_x emission rate. Point sources located within the modeling domain will be ranked and a cut-off emissions rate for use of the P-i-G treatment will be selected following a review of this information by the technical advisory group. The goal will be to accommodate all large point sources and as much of the elevated emissions as practicable.

Quality Assurance of the Emissions Inputs

Obviously, the accuracy and representativeness of any UAM-V modeling inventory will be limited by the quality of the input emissions data. Although the EPS 2.5 modules do perform some basic validity checks upon data input to each module, verifying the accuracy of the original emissions data is not a function of the EPS 2.5 system. Consequently, appropriate quality assurance procedures must be performed on the input emissions data prior to processing through EPS 2.5. Our proposed approach to quality assurance of the emissions inventory, which addresses both of these concerns, accordingly distinguishes between two basic levels of quality assurance. The first regards the inherent quality of the data input to EPS 2.5; the second pertains to tracking the data through each step of processing.

We will review the base year inventory database used to develop the UAM-V modeling inventories, along with any available documentation, and assess the methodologies, assumptions, emission factors, and other parameters used to estimate emissions to the extent that this information is available from existing documentation or internally documented within the inventory database. The quality review process will follow the guidance set forth in *Quality Review Guidelines for 1990 Base Year Emission Inventories* (EPA-454/R-92-007, August 1992). This document describes a two-tiered approach to quality review; SAI will employ a similar procedure in reviewing the base year inventory for the GCOS modeling domain. The Level I review will consist of an overall assessment of the inventory to ensure that the minimum data requirements and quality standards set forth in *Emission Inventory Requirements for Ozone State Implementation Plans* (EPA-450/4-91-010, March 1991) are met. The types of issues that will be addressed in the Level I review include the following:

- inclusion of all required components (i.e., point, area, on-road motor vehicles, biogenics)

- geographical coverage of the inventory (emission estimates should be provided for all counties in the modeling domain, not just the counties located in the actual or potential nonattainment area)

- assessment of completeness of database (identification of default or missing values for inventory parameters such as source location, stack parameters, operating schedules, etc.)

The two-tiered quality review process described above addresses the inherent quality of the data input to the EPS 2.5 system. The second phase of this effort will address the processing of the input inventory data to generate the base year UAM-V modeling inventory. To conduct this review, SAI will track the emissions data set through each stage of EPS 2.5 processing. SAI will verify that the specified input and output files for each processing step contain the appropriate information required to process the emissions data in the expected manner. Temporal profile assignments for each source category, including seasonal, weekly, and diurnal variations will be reviewed. The spatial allocation surrogate data and surrogate assignments for each source category will also be examined. SAI will ascertain that all required processing steps have been completed in an appropriate order and will track input and output emissions totals for each processing step to identify any gross errors in processing. For the future year modeling inventory, the review will focus on the control assumptions and projection factors used to estimate future year emission rates.

Each of the EPS 2.5 core modules and utilities produces a message output file containing summary information regarding the files processed, as well as indicating any error or warning conditions encountered during execution. These messages can be broadly categorized into three types: (1) messages pertaining to unsuccessful input/output (I/O) operations (i.e., opening, reading, and writing data files), (2) messages notifying the user that internal EPS 2.5 maximum parameters (which are used to dimension internal data arrays) have been exceeded, and (3) messages indicating invalid or questionable input data. SAI will examine the message files produced at each stage of processing to identify any warning or error conditions and reprocess data as needed to alleviate these conditions.

SAI will also make use of the quality control and reporting modules provided with EPS 2.5 as well as in-house quality assurance tools (e.g., plotting programs for examining temporal variations and spatial distribution of gridded emissions) to further examine the modeling inventory. Tabular summaries of speciated emissions by facility, SIC, and SCC for point sources and by ASC for area and on-road mobile sources will also be prepared to allow the ranking of individual sources and source categories with regard to ozone forming potential. This will facilitate identification of those sources that are particularly likely to have a significant impact on ozone formation in South Carolina, and specifically the areas of interest, because of the reactivity of the associated VOC emissions.

METEOROLOGICAL INPUT PREPARATION

Meteorological Input Requirements

The UAM-V requires hourly, gridded of wind, temperature, water-vapor concentration, pressure, vertical exchange coefficients (K_v), cloud-cover, and rainfall-rate. Meteorological inputs for this UAM-V application will be prepared using the MM5 meteorological model. All meteorological inputs will be directly specified for UAM-V Grids 1, 2, and 3 (refer to Figure 4-1 for the grid definitions). This section summarizes the preparation of meteorological inputs using the MM5 modeling system.

Meteorological Data

The UAM-V requires hourly, gridded of wind, temperature, water-vapor concentration, pressure, vertical exchange coefficients (K_v), cloud-cover, and rainfall-rate. Accurate representation of the day-specific meteorological conditions are critical to good model performance for UAM-V. For this we will depend upon the ability of the MM5 to provide physically realistic meteorological fields that represent the observed data, and will use our experience in the application of this model to appropriately specify the options and input parameters. Nevertheless, there will be some uncertainties inherent in the resulting meteorological fields. Thus, an important part of our job in this task is to evaluate the MM5.

Meteorological Modeling Tools and Procedures

A general description of the MM5 meteorological model is found in Anthes and Warner (1978). The governing equations include the equations of motion, the continuity equations for mass and water vapor, and the thermodynamic equation. Those features relevant to this application are briefly described in this section.

The current version of MM5 can be applied in a non-hydrostatic mode for the improved simulation of small-scale vertical motions (such as those associated with the sea breeze and terrain effects). Use of this optional feature can be important to the accurate simulation of the airflow and other features at high horizontal resolution and will be utilized for this study.

The MM5 model employs the sigma vertical coordinate: $\sigma = (p - p_t)/(p_s - p_t)$, where p is pressure, p_t is the constant pressure specified as the top of the modeling domain, and p_s is the surface pressure. The sigma-coordinate surfaces follow the variable terrain. Twenty vertical levels will be employed for this application such that the greatest vertical resolution is obtained within the boundary layer. Information on the vertical structure of the MM5 modeling domain is given in Table 4-1.

The governing equations are integrated over a grid that is staggered in the horizontal and vertical (Messinger and Arakawa, 1976). In the horizontal, the u and v wind components are calculated at points that are staggered with respect to those for all other variables. In the vertical, vertical velocity is defined at the sigma levels while all other variables are defined at intermediate sigma levels.

The MM5 modeling system also supports the use of multiple nested grids. This feature is designed to enable the simulation of any important synoptic scale features at courser resolution, while incorporating a high-resolution grid over the primary area(s) of interest. In this manner, the computational requirements associated with use of a high-resolution grid over a large domain are avoided. For this study, the MM5 modeling system will be applied for a much larger area than that used for the UAM-V modeling. The modeling domain was presented in Figure 4-2 and consists of an extended outer grid with approximately 108 km horizontal resolution and four inner (nested) grids with approximately 36, 12, and 4 km resolution, respectively. A Lambert Conformal map projection will be used for the application, to minimize the distortion of the grids within the area of interest. A one-way nesting procedure in which information from the simulation of each outer grid is used to provide boundary conditions for the inner grids will be employed.

To facilitate the realistic simulation of processes within the atmospheric boundary layer, variable surface parameters (including albedo, roughness length, and moisture availability) and a high-resolution planetary boundary layer (PBL) parameterization will be used for the simulations. The PBL parameterization also requires use of a multi-layer soil temperature model (an otherwise optional feature of MM5).

For the coarse grids, the Kain-Fritsch cumulus parameterization scheme (Kain and Fritsch, 1990) will be used to parameterize the effects of convection on the simulated environment. This feature will not be employed for the high resolution grids (AB and C) where an explicit moisture scheme (stable precipitation) will be used.

The MM5 model supports four-dimensional data assimilation (FDDA), a procedure by which observed data are incorporated into the simulation. FDDA option include (1) “analysis nudging” in which the simulation variables are relaxed or “nudged” toward an objective analysis that incorporates the observed data and (2) “obs nudging” in which the variables are nudged toward individual observations. These two approaches to FDDA are described in some detail by Stauffer and Seaman (1990) and Stauffer et al. (1991). For this study, analysis nudging will be used for all variables.

The data for preparation of the terrain, initial and boundary condition, and FDDA input files for this application will be obtained from NCAR. The MM5 input files will be prepared using the preprocessor programs that are part of the MM5 modeling system (Gill, 1992).

The MM5 modeling system was recently modified to include the output of the internally calculated vertical exchange coefficients (K_v). The K_v values are intended to represent non-local or multi-scale diffusion coefficients (rather than local diffusion coefficients) as described by (Hong and Pan, 1995). This information will be used to specify the vertical exchange coefficients required by the UAM-V modeling system.

For each simulation period, the model will be initialized at 0000 GMT on the first day of the period. Thus, the MM5 simulation period will include a five-hour initialization period, before the output will be used to prepare inputs for the UAM-V model. For the three outer grids, the MM5 will be run continuously for the nine-day simulation period. For the higher-resolution grids, the model will be reinitialized after each three days of simulation. Each reinitialization will also include an additional 5-hour initialization period. Reinitialization times may vary based on a review of the simulation results. The input fields from each simulation will be inspected to ensure that piecing together the simulations does not create discontinuities in the meteorological inputs (the use of FDDA will alleviate this possibility).

The time step used for the simulations will range from several minutes for the outermost (approximately 108 km) grid to approximately 12 seconds for the innermost (approximately 4 km) grid.

The MM5 output will be postprocessed to correspond to the UAM-V modeling domain and the units and formats required by the modeling system using the MM52UAMV postprocessing software. Wind, temperature, water-vapor concentration, pressure, vertical exchange coefficient, cloud-cover, and rainfall-rate input files containing hourly, gridded estimates of these variables will be derived from the MM5 output. Surface temperature and solar radiation will be postprocessed for use in preparing the mobile-source and biogenic emissions estimates.

Quality Assurance of the Meteorological Inputs

The MM5 simulation results will be evaluated using graphical and statistical analysis. A list of graphical and statistical products is included at the end of this section. The overall evaluation of the MM5 results will include the following elements. For the outer grids, examination of the MM5 output will focus on representation of the regional-scale meteorological features and airflow patterns and will include a comparison with weather maps as well as the items listed below. A more detailed evaluation of the results for the inner (high-resolution) grid will emphasize representation of the observed data, terrain-induced and other local meteorological features, and vertical mixing parameters. To the extent possible, the modeling results will be compared with observed data. In the absence of data, they will be examined for physical reasonableness as well as spatial and temporal consistency. Since data assimilation will be used, a comparison with the observed data primarily serves as a check on the data assimilation but can also reveal potential bias in the meteorological inputs. The ability of the MM5 model to reproduce observed precipitation patterns will be qualitatively assessed by comparing the simulated and observed rainfall patterns (based on NWS data). A detailed analysis of the timing and amount of the precipitation will not be performed.

The UAM-V ready meteorological inputs will also be plotted and examined to ensure that the characteristics and features present in the MM5 output are retained following the postprocessing step.

The following graphical summaries will be prepared to facilitate the review/evaluation of the meteorological inputs:

- 3-dimensional visualizations of the MM5 output using the WXPortal software (an enhanced version of VIS-5D)

- x-y cross-section plots of the MM5 wind fields for several levels and times with observations overplotted for MM5 Grids 1, 2, and 3

- x-y cross-section plots of the UAM-V ready wind, temperature, water-vapor concentration, vertical exchange coefficient, cloud-cover, and rainfall-rate fields for several times and levels (as appropriate)

- plots of the UAM-V ready vertical profiles of K_v for selected locations (four times per day)

Following the initial application of UAM-V for each simulation period, the MM5 results will be further reviewed/evaluated using the UAM-V process analysis technique. This technique allows one to examine the meteorological features in relation to their effects on the UAM-V simulation results. The ability of the meteorological model to simulate features such as the sea breeze, can also be assessed by examining whether the signature appears in the ozone concentration patterns.

As an example, we used process analysis for the first GCOS simulation period and found that the MM5 tended to underestimate the wind speeds during certain of the simulation days. The very light winds effectively turned off the deposition term. In this manner, process analysis was used to detect and correct problems with the meteorological inputs. We will use process analysis in this study to similarly guide the diagnostic analysis of the UAM-V simulation results. This may lead to refinement of the meteorological inputs.

AIR QUALITY INPUT PREPARATION

Air Quality Input Requirements

There are three UAM-V air quality input files that define pollutant concentrations for each of the UAM-V state species (1) throughout the three-dimensional grid at the initial simulation time (coarse-grid only), (2) along the lateral boundaries of the modeling domain for each hour of the simulation period, and (3) along the top of the modeling domain for the entire simulation period.

Air Quality Data

For each simulation period, pollutant concentration data for all monitoring sites located within the modeling domain will be obtained from the EPA Aerometric Information Retrieval System (AIRS) and will be supplemented (if possible) with data from CASTNET. Species will include ozone, NO, NO_2, CO, and hydrocarbons. Estimates of background concentrations of the various pollutants will be obtained from EPA (1991).

Air Quality Input Preparation Tools and Procedures

Preparation of the initial and boundary condition input files will entail the application of the air quality preprocessor programs included as part of the UAM-V modeling system. The model will be initialized at 0000 EST on the first day of each simulation period. Initial conditions will be obtained through the interpolation of observed data. To avoid the unrealistic interpolation of the observed data to unmonitored areas, pseudo sites with background pollutant concentrations may be placed in these area to provide more complete geographical coverage for the interpolation; the resulting dataset used in the interpolation will consist of both actual and pseudo monitors. The surface-based values will be used for the surface layer and will be used to calculate the concentrations within each model layer using theoretical profiles

The primary reason for using a nested-grid, regional-scale modeling configuration is to reduce the uncertainty in the boundary conditions for the area of interest. In this case, lateral boundary conditions need only be specified for the outermost (coarse-grid) domain. Top boundary conditions are specified for all domains in a single file. For this study, the lateral and top boundary concentrations for all pollutants will be set equal to constant values. The lack of pollutant concentration data (especially aloft) as well as the length of the simulation periods precludes a more detailed specification of the boundary conditions. Precursor will be set to continental background or maritime background values as appropriate. Ozone will specified using a new “self-generating” ozone boundary condition technique developed by SAI for the GCOS modeling analysis. This technique makes use of the modeling results to calculate a domain-wide average concentration (aloft) for each simulation day. This value is then used to specify the ozone concentrations for the subsequent day. Use of this technique precludes the need to specify alternate future-year boundary conditions – as the UAM-V will also provide this information.

Given the expected geographical extent of the modeling domain beyond the primary areas of interest, the coarse-grid boundary conditions are not expected to significantly influence the simulation results within the area of interest. This assumption may be tested as part of the modeling analysis.

Quality Assurance of the Air Quality Inputs

Plots of the initial conditions for ozone, NO, NO_2, CO, and selected hydrocarbon species, and tabular summaries of the boundary condition values will be prepared. Stepwise quality assurance of the air quality input preparation procedures will also be conducted

LAND-USE INPUT PREPARATION

Land-Use Input Requirements

A gridded land-use file is required for the full domain and each subdomain.

Land-Use Data

The surface characteristics file will be prepared using the latest available 200-m resolution land-use data obtained from the U.S. Geological Survey (USGS). Each of the categories in the USGS land-use database will be assigned to one of the 11 UAM-V categories. These include urban, agricultural, range, deciduous forest, coniferous forest (including wetlands), mixed forest, water, barren land, non-forest wetlands, mixed agricultural and range, and rocky (low shrubs).

Land-Use Tools and Procedures

Preparation of the land-use input files (for the full domain and each subdomain) will entail the application of the land-use preprocessor program included as part of the UAM-V modeling system. The 200-m resolution data are aggregated to the grid cells and the percent distribution among the categories is calculated. The resulting distribution for grid cells along the South Carolina coast will be carefully examined and refined, as needed, to better reflect the high-resolution data along the land-water boundary.

Quality Assurance of the Land-Use Inputs

Plots of the percentage distribution of land-use for each of the 11 land-use categories will be prepared and examined. Stepwise quality assurance of the land-use input preparation procedures will also be conducted.

CHEMISTRY INPUT PREPARATION

Chemistry Input Requirements

Application of the UAM-V modeling system requires preparation of several additional input files that contain information on albedo, ozone column, photolysis rates, and chemical reaction rates. This information is required for the full domain and each subdomain.

Ozone Column Data

For each simulation period, day-specific ozone column data will be obtained from the National Aeronautics and Space Administration (NASA).

Chemistry Related Input Tools and Procedures

Preparation of the chemistry related input files will entail the application of the standard preprocessor programs included as part of the UAM-V modeling system. The range of ozone column values for the entire domain for each simulation period will be calculated for use in the photolysis rates preprocessor program. The haze parameter for UAM-V (aerosol optical depth) will be set to 0.094 (a value typical of rural conditions) for the entire modeling domain. Albedo will be specified according to land-use type (based on information contained in the surface file) by the albedo/haze/ozone column processor.

Chemical reaction rates, activation energies, and maximum/minimum species concentrations, as used in the validation of the CBM-IV chemical mechanism against smog chamber data, will be utilized along with appropriate updates for the enhanced treatment of radical-radical termination reactions and isoprene chemistry.

Photolysis rates will be calculated using JCALC preprocessor program, utilizing the values of albedo, haze, and total ozone column information discussed above.

Quality Assurance of the Chemistry Related Inputs

The ozone column values and photolysis rates will be tabulated and examined. Stepwise quality assurance of the chemistry related input preparation procedures will also be conducted.

6 MODEL PERFORMANCE EVALUATION

A typical application of the UAM-V modeling system for ozone air quality assessment purposes consists of several simulations, including an initial simulation and a series of diagnostic and sensitivity simulations (designed to examine the effects of uncertainties in the inputs on the simulation results, identify deficiencies in the inputs, and investigate the sensitivity of the modeling system to changes in the inputs). For each simulation, model performance is primarily assessed through graphical and statistical comparison of the simulated pollutant concentrations with observed data. The results of this comparison are used to guide the modeling analysis (through the determination of additional diagnostic and sensitivity simulations) and to assess whether the model is able to adequately replicate the air quality characteristics of the simulation period. Model performance evaluation tests and procedures are described in this section. Diagnostic and sensitivity analyses that may be performed to understand and improve model performance are discussed in Section 7.

EPA guidance (EPA, 1999a) stresses the need to evaluate the model relative to how it will be used in the attainment demonstration; that is in simulating the response to changes in emissions. Various aspects of the model performance evaluation, such as assessment of the ability of the model to simulate weekday-weekend differences in concentration levels and patterns, detailed evaluation of the changes in process-level contributions, and comparison with air quality and emissions trends will be used to evaluate the reliability of the modeled response.

Once acceptable model performance is achieved (based on the results of the graphical, statistical, and sensitivity analysis), the simulation is subsequently referred to as the base-case simulation. The establishment of a base-case simulation is integral to the reliable use of the modeling system to assess the effects of changes in emissions on future air quality.

This section of the protocol document describes the procedures to be used to evaluate model performance.

MODEL PERFORMANCE DATA

Data from all air quality monitoring sites within the South Carolina modeling domain will be used in the evaluation of model performance. For the most part, these include measurements of ozone, NO, NO_2, NO_x, and CO for routine monitoring sites (including photochemical assessment monitoring sites, PAMS) located throughout the region (and primarily in the urban/nonattainment areas). These data will be obtained from AIRS. We will supplement this database, if possible, with data from the CASTNET and SCION monitoring program. Several CASTNET and SCION monitors are located throughout the Southeast. Data from these sites will typically include higher resolution NO_x measurements (compared to the routine monitoring sites) and may also include measurements of hydrocarbon species. Data from special studies commensurate with the simulation periods will also be solicited and incorporated as time and resources permit. Note that the analysis and use of special-study data can sometimes be very resource intensive.

An analysis of the observed data will be performed to develop a detailed description of the ozone episode characteristics for use in the model performance evaluation.

MODEL PERFORMANCE OBJECTIVES

As noted earlier, the overall objective of a model performance evaluation is to establish that the modeling system can be used reliably to predict the effects of changes in emission reductions on future-year ozone air quality and to evaluate the effectiveness of possible attainment demonstration strategies. Specific objectives for this study include: (1) ensuring that the regional-scale modeling results provide appropriate boundary conditions for the primary areas of interest, (2) ensuring that the ozone concentration patterns and levels and the day-to-day variations in these are accurately represented, and (3) ensuring that the modeling system exhibits a reasonable response to changes in the inputs (and that the inputs do not contain significant biases or compensating errors).

MODEL PERFORMANCE EVALUATION PROCEDURES

The evaluation of model performance will follow the general procedures outlined in this section. Variations to these may be proposed and incorporated during the course of the study to address specific issues that arise. All additions/changes will be discussed with the SC DHEC.

Model Performance Evaluation Components

The evaluation of model performance will include both qualitative and quantitative components. For each simulation conducted as part of the base-case modeling analysis, a variety of graphical and statistical analysis products will be prepared. These are listed and described in the remainder of this section and will provide the basis for the model performance evaluation. The analysis and integration of these results, relative to the objectives (as given earlier in this section), will complete the evaluation of model performance.

Geographical Considerations

The simulation results for the full domain and each subdomain will be examined using a variety of graphics, metrics, and statistics (these are summarized later in this section). Analysis of results for the coarse-grid (36 and 12-km resolution) domains will emphasize representation of the regional-scale concentration levels and patterns, as well as day-to-day variations in regional-scale air quality. Statistics will be calculated for the coarser grids, but are not expected to be very meaningful for the scale represented by these grids. A more detailed analysis of the results will be performed for the high-resolution (4-km) grid. This will include the analysis of the magnitude and timing of site-specific concentrations (1-hour and 8-hour), a more rigorous statistical evaluation (compared to the coarser grids), and the use of process analysis.

Temporal Considerations

The ability of the modeling system to depict the day-to-day differences in ozone concentration, as indicted by the observations, will be examined for each domain and episode period. Diurnal variations in ozone for the coarser grids will be examined relative to the boundary condition estimates for the finer grids. Site-specific, hourly variations for ozone and precursor species will be examined (using time-series plots and statistical measures) for sites within the high-resolution domains.

The analysis of model performance will focus on 1-hour concentrations of ozone and other species, since the data are typically reported as hourly values. However, the ability of the model to represent maximum 8-hour ozone concentration is related to its ability to represent the hourly values that comprise the 8-hour maximum. Thus, a comparison of maximum 8-hour average ozone concentration will also be performed for the high-resolution grids.

Species

All relevant species represented by the observed data within the high-resolution domains will be included in the model performance evaluation. We will also consider the calculation of ratios or other derived parameters.

Summary of Graphical Displays, Metrics, and Statistical Parameters

Graphical displays and statistical/tabular summaries of the UAM-V simulation results will provide the basis for model performance evaluation and will be used to guide the interpretation and use of the UAM-V simulation results. For each simulation performed as part of the base-case modeling analysis, the graphical displays and tabular summaries will include:

- Isopleth plots of daily maximum simulated ozone concentration (1-hour and 8-hour), with observed values overplotted for all UAM-V grids

- Time-series plots (with range shading) of hourly ozone, NO, NO_2, NO_x, VOC, and CO concentrations for each monitoring site (and possibly other unmonitored locations) within the high-resolution grids

- Scatter plots of hourly ozone, NO, NO_2, NO_x, VOC, and CO concentrations (and possibly selected indicator species) for each UAM-V grid

- Scatter plots of 8-hour maximum ozone concentration for each UAM-V grid

- Scatter plots comparing the time of the simulated and observed 8-hour maximum ozone concentrations for each monitoring site within the high-resolution grids

- More than 20 metrics and performance statistics[4] for ozone, NO, NO_2, NO_x, VOC, and CO (these include various maximum, minimum, mean, accuracy, bias, error, residual, and ratio-based parameters as well as the EPA-recommended measures for 8-hour ozone model performance that focus on the use of maximum 8-hour values near the monitoring site averaged over all sites or for each site over all simulation days)

- Time-series plots of selected metrics and statistics for ozone (and other pollutants as appropriate) for all UAM-V grids

- Animations of simulated ozone concentrations for selected grids/levels (and selected simulations)

These plots and tabular summaries will be used to display/convey the results of a single simulation or to compare two different simulations, as appropriate. In the latter case, the plots and animations may be presented as concentration differences.

If the UAM-V process-analysis technique is employed for a given simulation, the process-analysis results (for ozone, NO_x, and VOC) will be displayed using SAI's standard 3-panel plots, which show the hourly contribution (separately and cumulatively) and the daily net contribution for each simulation process. These will be used to display the results of a single simulation or to compare two different simulations, as appropriate.

DETERMINATION OF ACCEPTABLE MODEL PERFORMANCE

An integrated assessment of the above information (obtained as part of the base-case modeling analysis) will be used to document and qualitatively and quantitatively assess whether an acceptable base-case simulation has been achieved. Certain of the statistical measures will be compared to the EPA recommended ranges for acceptable model performance for urban-scale photochemical model applications. EPA has provided ranges for three key statistical measures for 1-hour ozone. The measures and recommended ranges are as follows: unpaired accuracy of the peak concentration (± 20 percent), normalized bias (± 15 percent), and normalized gross error (35 percent). We will also examine the average accuracy of the peak concentration and compare this with the range for the unpaired accuracy. These criteria are most applicable for the assessment of model performance for the high-resolution grid and/or selected urban-scale subregions thereof. However, they will also be used to guide the assessment of model performance for the regional-scale domains (Grids 1 and 2). The additional statistical measures recommended by EPA in the draft guidance for 8-hour ozone modeling will also be calculated and compared with the recommended ranges. These include the domain-wide average accuracy of the 8-hour ozone peak and the site-specific average accuracy of the peak over all simulation days. The recommended range for both of these measures is ± 20 percent. The 8-hour statistics will be calculated for the high-resolution grid and selected subregions only.

---

[4] These are listed in Table 6-1.

USE OF MODEL PERFORMANCE RESULTS TO GUIDE THE INTERPRETATION AND USE OF MODELING RESULTS IN THE ATTAINMENT DEMONSTRATION

Information obtained as part of the model performance evaluation can be used to guide the interpretation and use of the results in the attainment demonstration. A simple example of such use is the case where ozone concentrations are overestimated for one or more sites in the base-case simulation. It is possible that the overestimation could affect the response of the modeling system to emissions changes. If the site(s) for which ozone is overestimated show a different result in the attainment demonstration than most other sites, and there are no other apparent reasons for these differences, the overestimation might explain the different response. This would be further examined and possibly offered as "weight of evidence". As a second example, differences in model performance among days or episodes might cause a different weighting of the results in the attainment demonstration analysis.

TABLE 6-1. Standard list of UAM-V simulation metrics and performance statistics.

Number of data pairs
Maximum domain-wide simulated value
Max station-wide sim value
Maximum observed value
Domain-wide unpaired accuracy
Station-wide unpaired accuracy
Average accuracy of peak
Normalized bias
Normalized gross error
Fractional bias
Fractional gross error
Ratio of bias to mean observation
Ratio gross error to mean observation
Maximum residual
Minimum residual
Mean unsigned error
Mean residual
Mean simulated value
Mean observation
Root mean square error
Standard deviation of fractional bias

7 DIAGNOSTIC AND SENSITIVITY ANALYSIS

In accordance with EPA guidance, diagnostic and sensitivity analysis will be used in this study to:

- better understand the simulation results
- obtain information that will help to prioritize efforts to improve/refine model inputs
- obtain insights in the effectiveness of various control strategies
- assess the "robustness" of a control strategy

The first two bullet items pertain to the base-case modeling analysis and are addressed in this section of the protocol document. The latter two items pertain to the future-year analysis and are addressed in Sections 8 and 9, respectively.

The type of diagnostic and sensitivity simulations performed as part of the base-case modeling effort will be based on the inputs and/or assumptions used in preparing the inputs and the simulation results (for the initial and diagnostic/sensitivity simulations). They will include simulations incorporating modification or refinement of the inputs as well as a detailed analysis of the simulation processes (using the process analysis feature of UAM-V).

DETERMINATION OF APPROPRIATE DIAGNOSTIC/SENSITIVITY SIMULATIONS

The exact simulations to be performed for each simulation period will be determined based on a review of the initial (and subsequent diagnostic/sensitivity) simulations results or knowledge of sources of uncertainty in the inputs. A total of eight diagnostic/sensitivity simulations will be performed for the selected simulation period. Design of the simulations will consider the eventual use of the modeling results in the relative sense (in the attainment demonstration). Specification of the diagnostic and sensitivity simulations will be made in conjunction with SC DHEC. These may include, for example, modification of the emissions or meteorological inputs or use of alternative input parameters. Simulations or analyses (e.g. calculation of boundary fluxes) may also be designed to assess the effects of inter- or intra-regional transport.

DIAGNOSTIC/SENSITIVITY ANALYSIS PROCEDURES

All diagnostic and sensitivity simulations will be conducted using the general procedures outlined in Section 5 and 6 of the protocol document. Per EPA guidance, adjustment to the inputs to improve model performance will be within reasonable bounds. Review of the results will consider the possible effects of any modifications on the calculation of relative reduction factors in the attainment demonstration.

USE OF THE DIAGNOSTIC/SENSITIVITY ANALYSIS RESULTS

The results of the diagnostic and sensitivity analyses may be used to (1) modify or enhance inputs, (2) improve model performance, and (3) guide the interpretation and use of the modeling results in the attainment demonstration. Errors in the inputs that are uncovered as part of the diagnostic/sensitivity analysis will be documented and corrected. Adjustment to the inputs to accommodate uncertainty will be within reasonable bounds and will not be commensurate with poorer model performance (EPA, 1999a). For example, as noted in Section 5, the UAM-V results may indicate that additional review of the meteorological inputs, re-application of the MM5, or re-postprocessing of the MM5 output is required. All such modifications/adjustments to the inputs will be technically justifiable, and will be documented. Finally, information obtained as part of the diagnostic/sensitivity analysis can be used to guide the interpretation and use of the results in the attainment demonstration.

8 FUTURE-YEAR MODELING

Once an acceptable base-case has been achieved, the UAM-V can be used to predict future-year air quality and to evaluate the effectiveness of attainment strategies. In this section, we summarize the procedures to be followed in conducting future-year modeling for the South Carolina areas of interest. As noted earlier in the protocol document, SAI will prepare the future-year baseline inventory while the remainder of the work will be conducted by SC DHEC, with guidance and assistance from SAI (as needed).

SELECTION OF A FUTURE YEAR

The future-year for the baseline modeling will be 2007 to demonstrate attainment for South Carolina's Early Action Compact. SC DHEC will also demonstrate that the control strategies developed to show compliance for 2007 will be sufficient to maintain compliance in future years. The future-year of 2012 has been selected for this purpose. Data for the future year of 2010 will also be provided, since this data will be available from preliminary modeling work.

FUTURE-YEAR EMISSION INVENTORY PREPARATION

Projection inventories are necessary to determine whether a given area will achieve or exceed the ozone standard in future years. There are basically two types of projections: baseline projections and control strategy projections. Baseline projections are estimates of future year emissions that account for both expected growth in an area and air pollution control regulations that are in effect at the time the projections are made. Note that certain provisions in existing control regulations may take effect only at some future date, and baseline projections should include the effects of these expected changes. By contrast, control strategy projections also include the expected impact of revised or additional control regulations.

To prepare the future baseline inventory, we will apply growth and control factors to the base-year emission inventory. For GCOS, we have used Bureau of Economic Analysis (BEA) estimates of gross state product and employment to project growth and information supplied by EPA to represent national controls. For ATMOS, we are using the EGAS system. If more state- or area specific data are available for use in this study, we will obtain these from the State and use this instead. In the absence of state-specific data, default growth projections prepared by the Bureau of Economic Analysis will be applied based on 2-digit SIC code for point sources and on the EPS 2.5 default projection factor assignments by source category code for area and mobile sources. The control factors to be applied will represent reductions in emissions that should occur as a result of existing control regulations. Again, state-specific data will be used to the extent available. In the absence of state-specific data, default controls based on information provided by EPA will be applied. Note that EPA guidance recommends that future year modeling inventories be based on allowable emission rates rather than actual. The 1996 NET inventory which will be used in this study does not include allowable emissions data; in some cases, this information may only be available from state or local air permit files. Consequently, we will also obtain any source-specific allowable emissions data to be used for the modeling.

The future-year baseline emissions inventory will be prepared in accordance with EPA guidance, *Emissions Inventory Guidance for Implementation of Ozone and Particulate Matter National Ambient Air Quality Standards (NAAQS) and Regional Haze Regulations* (EPA, 1999b), and will incorporate emission reductions associated with the NO_x SIP Call and the Tier II low-sulfur fuels and vehicle standards program.

SPECIFICATION OF OTHER INPUTS FOR FUTURE-YEAR SIMULATIONS

With the exception of the emission inventories and the boundary conditions, all inputs for the future-year simulations will be identical to those for the corresponding base-case simulation. The modeling emission inventories will be developed explicitly for the future year and scenario. The self-generating ozone boundary condition technique will be used for specification of the future-year boundary conditions.

FUTURE-YEAR MODELING

Once an acceptable base-case has been achieved, the UAM-V can be used to predict future-year air quality and to evaluate the effectiveness of attainment strategies. In this section, we summarize the proposed approach to conducting the future-year baseline modeling.

Future-Year Baseline Simulation

The overall objective of the future-year modeling exercises is to evaluate the likelihood of future-year compliance with the 8-hour ozone NAAQS and, as necessary, assess the effectiveness of various control strategies to improve ozone air quality in the three focus areas. An important component of this is the establishment of a future-year baseline simulation.

The future-year baseline emission inventory will incorporate the effects of population and industry growth (or, in some cases, decline) as well as national or state-wide control measures or programs that are currently expected to be in place by the selected future year date. Projection to the future-year for the baseline simulation will include emissions for the entire modeling domain. The baseline simulation results provide the starting point for assessment of the effects of further emission reductions on future ozone air quality. In this task, we will conduct UAM-V modeling using the future-year baseline emissions inventory, compare the results with the base-case simulation, and perform a preliminary assessment of the results using the EPA 8-hour ozone attainment demonstration procedures. The review, comparison, and preliminary assessment of results will include graphical displays, animations, and preparation of an ACCESS™ Database for Visualizing and Investigating Strategies for Ozone Reduction (ADVISOR).

Emissions-Based Sensitivity Simulations

The discussion in the remainder of this section refers to work that will most likely be conducted by SC DHEC, with guidance and assistance from SAI (as needed).

One of the objectives of the future-year modeling exercises is to evaluate the likelihood of future-year compliance with the 8-hour ozone NAAQS and, as necessary, assess the effectiveness of various effective control strategies to improve ozone air quality in South Carolina, and specifically, the areas of interest. This will be accomplished by first conducting a series of emission sensitivity simulations.

The sensitivity analysis will involve an initial set of simulations reflecting simple, across-the-board emission reductions from the established 2007 baseline inventory. The modeling effort may include a number of across-the-board emission sensitivity simulations involving varying reductions in VOC and NO_x emissions. An example set of sensitivity simulations is as follows:

- 15 percent reduction in anthropogenic VOC emissions
- 15 percent reduction in anthropogenic NO_x emissions
- 35 percent reduction in anthropogenic VOC emissions
- 35 percent reduction in anthropogenic NO_x emissions
- 15 percent reduction in anthropogenic VOC emissions and 35 percent reduction in anthropogenic NO_x emissions
- 35 percent reduction in anthropogenic VOC emissions and 15 percent reduction in anthropogenic NO_x emissions
- 35 percent reduction in anthropogenic VOC and NO_x emissions

The results of the emission sensitivity simulations will be compared with the 2007 baseline simulation results using difference plots and through comparison of the metrics to determine the relative effectiveness of the different types and amounts of emission reductions, as well as any synergistic effects (i.e., the decrease in maximum 8-hour ozone concentration obtained from the combined VOC and NO_x reductions may be greater than the sum of the decreases when the emission reductions are applied separately).

Control-Strategy Simulations

On the basis of the results of the emission reduction sensitivity modeling, control strategy options will be identified, simulated, and evaluated in this task. Draft guidance for demonstrating attainment of the 8-hour NAAQS has been developed by EPA. This guidance will provide the methodologies to be followed in conducting a modeling attainment demonstration, as described in more detail in Section 9 of the protocol document.

The control scenarios to be simulated will likely involve a combination of reductions from all source sectors including mobile, area, and point sources. The various options can be evaluated in terms of the cost effectiveness of reducing future-year ozone concentrations. The simulation results will be presented with the graphical and statistical tools used for the sensitivity modeling analysis. Special products will be prepared, if necessary, to meet the reporting requirements for the attainment demonstration exercise as outlined in the EPA guidance document.

DISPLAY AND PRESENTATION OF FUTURE-YEAR SIMULATION RESULTS

Graphical displays and statistical/tabular summaries of the UAM-V simulation results will also provide the basis for the review and preliminary assessment of future-year baseline simulation results. The graphical displays and tabular summaries will include:

- Isopleth and isopleth difference plots of daily maximum simulated ozone concentration, with observed values overplotted for the 12 and 4 km UAM-V grids

- Animations of simulated ozone concentrations and concentration differences for selected levels (and selected simulations)

- Interactive ADVISOR database containing information for review, comparison, and assessment of the simulation results. The database will contain both emissions and simulated ozone concentrations (as represented by several different metrics) for selected regions and subregions of the domain, for both the base-case and baseline simulations. Users will be able to view (and extract) the data in spreadsheet format and to create plots, the contents of which will reflect various user-specified options.

  Metrics will include:
  - maximum 1-hour ozone concentration (ppb)
  - maximum 8-hour ozone concentration (ppb)
  - number of grid cell · hours with maximum 8-hour ozone concentrations ≥ 85 ppb
  - total ozone exposure (ppb · grid cell · hour)
  - exceedance ozone exposure (ppb · grid cell · hour) for concentrations ≥ 85 ppb
  - population exposure (to concentrations ≥ 85 ppb)
  - total emissions (NO_x, VOC)

  Options for displaying the metrics will include:
  - value
  - difference (relative to a selected base simulation such as the future-year baseline)
  - effectiveness (change in ozone metric relative to the change in emissions, again relative to a selected base simulation)
  - relative reduction factor (for the site-specific geographies only)
  - estimated design value (for the site-specific geographies only)

Geographies will include:

- 12 and 4 km modeling grids
- State of South Carolina
- Anderson/Greenville/Spartanburg area counties
- Aiken/Columbia area counties
- Darlington/Florence area counties
- Rock Hill area counties
- all monitoring sites in South Carolina

ADVISOR also allows application of the new EPA attainment demonstration procedures on a site-specific basis. Please visit the SAI UAM-V web site at http:\\uamv.saintl.com to download and review a demonstration version of the ADVISOR database. SAI has assisted SC DHEC in setting up an ADVISOR database. SC DHEC will be able to add the results of additional future-year emission sensitivity and control-strategy simulations to the ADVISOR database and thus use this tool to facilitate and enhance their review, analysis, and distribution of modeling results. ADVISOR runs on any PC and is a very effective way to distribute modeling results for independent analysis and interpretation.

9 ATTAINMENT DEMONSTRATION

At present it is anticipated that an attainment demonstration analysis will be conducted for the South Carolina modeling study and will include application of the new modeled attainment test as presented in the draft EPA guidance (EPA, 1999a) as well as other corroborative analyses. The specific procedures may change if the final EPA guidance is different from the draft guidance. Application of the draft procedures will provide a starting point for the assessment of the emissions changes that may be needed to achieve the currently proposed standard. These procedures are outlined in this section of the protocol document. Given that the results of the modeling analysis are unknown at this time, the details of the corroborative analyses cannot be specified. However, the general approach to identifying and conducting such analyses is presented. The present modeling analysis includes the preparation of the ADVISOR database to support the application of the attainment demonstration procedures.

The discussion in this section refers to work that will most likely be conducted by SC DHEC, with guidance and assistance from SAI (as needed).

GEOGRAPHICAL CONSIDERATIONS

The South Carolina ADVISOR database and associated analysis procedures outlined in this and the previous section are designed to support a separate 8-hour ozone assessment for each of the areas of interest (as required by the pending nonattainment designations). The current list of areas includes Anderson/Greenville/Spartanburg/Aiken/Columbia, Florence/Darlington, and Rock Hill. For each area of interest, the analysis will include the modeled attainment test, any requisite screening tests, and additional corroborative analysis.

MODELED ATTAINMENT TEST

The modeled attainment test as described in the draft EPA guidance on 8-hour ozone attainment demonstrations (EPA, 1999a) will be included along with all base- and future-year simulation results in the South Carolina ADVISOR database. Key implementation issues are presented and discussed in this section.

An important component of the attainment test is the calculation of a relative reduction factors (RRF) for each site and each simulation day, for each relevant (attainment demonstration) simulation. The RRF represents the ratio of the future-year daily maximum 8-hour ozone concentration to the corresponding base-year value. It is calculated for each site using simulated ozone concentrations within the “vicinity” of the site. For the South Carolina modeling application, “vicinity” will be defined based on analysis of the representativeness of the various monitoring sites. This analysis will examine emissions gradients, simulated concentration gradients, possible influence of geographical features, and model performance considerations.

Draft EPA guidance recommends the use of a 15-km radius of influence. It is possible that the use of a more limited radius of influence would better accommodate the geographic and meteorological variability influencing the observed and simulated ozone concentrations and would better preserve the site-specific nature of the attainment-demonstration exercise by ensuring that the sites are considered independently from one another. The radius of influence should also be defined in a manner that is consistent with standard model performance practices that require that accommodate very little displacement of the simulated peaks relative to the monitoring sites.

The RRF for a given monitor will be calculated using the grid-cell level simulated maximum 8-hour ozone concentration in the vicinity of the monitor. The grid cell containing this value may be different for the base year and the future year, since changes in emissions can alter the timing of the chemistry and the location of the maximum value. This approach is also consistent with the use of a high-resolution grid, since relocation of the maximum to a different grid cell in the vicinity of a monitoring site will not represent a large spatial shift.

The RRF can be calculated for a single day or as an average over multiple days. The ADVISOR database is designed to allow the user to specify which simulation days will be included in the calculation of the RRF. The user may select the day(s) directly or use one of three "automated" day selection options. These include (1) for each simulation day for which the simulated maximum 8-hour ozone value is greater than a user-specified value (including the EPA recommended default of 70 ppb), (2) for all observed 8-hour ozone exceedance days, and (3) for all days for which the base-case simulation results are within a user-specified range of model performance.

The estimated design value (EDV) for each site is then calculated by multiplying the RRF by the site-specific design value. The design value used will be the maximum of the design value that represents the 1998 episode (1999) or the value used for 8-hr ozone designations (2003). Use of the 1999 design value represents years 1997 – 1999 and is consistent with date of the episode and thus representative of the "current" year of 1998, as used for the base-case modeling. Use of the 2003 design value represents years 2001 – 2003 and is consistent with the EPA planned period for designation of 8-hour ozone nonattainment areas. Use of the maximum of the two values represents the most conservative approach and most closely follows the approach outlined in the EPA guidance.

SCREENING TEST

For unmonitored areas within the modeling domain that consistently exhibit simulated exceedances of the 8-hour NAAQS, the EPA recommended screening test will be applied. To apply the screening test to the South Carolina modeling domain, we will first define subregions within the domain (encompassing each potential 8-hour ozone nonattainment area). Within these subregions, we will then adopt the EPA definition of "consistently"[5] to identify locations for application of the screening test. The screening test will be applied

[5] Daily maximum 8-hour daily ozone at the location in question is more than five percent higher than near any monitored location on 50 percent or more of the modeled days.

using the mean design value for the subregion in which the unmonitored-area exceedance is consistently simulated. The predicted future design value for each area will then be the maximum of the values for all monitored and unmonitored "sites" within the subregion or area. If this value is less than 85 ppb, the test is passed.

OTHER COMPONENTS OF THE WEIGHT OF EVIDENCE DETERMINATION

If the modeled attainment and screening tests are passed or nearly passed, states may opt to include additional analyses as part of a "weight of evidence" determination. Current EPA guidance does not encourage a weight of evidence determination if the predicted design value for a given area is greater than or equal to 90 ppb. The specific analyses to be performed for each area will be determined based on the findings and results of the modeling analysis as well as a review of available data and information. EPA (1999a) suggests some core analyses. However, the currently available air quality data do not support the reliable use of observation-based models.

Per EPA guidance, the weight of evidence analysis will include additional analysis of the model output for each nonattainment area including (1) relative change in grid-cell-hours with maximum 1-hour ozone concentrations greater than or equal to 125 ppb and (2) relative change in the number of grid cells with 8-hour ozone concentrations greater than or equal to 85 ppb. Note that each of these will be included in the ADVISOR databases described in Section 8. A large reduction in these metrics would support a weight of evidence argument. In all cases, EPA guidance suggests that a value of 80 percent should be considered to be a large reduction.

A primary objective of the weight of evidence analyses is to use other methods to corroborate the modeling results or to independently assess the potential for attainment. Considerations in designing these analyses include:

- potential or expected effects of model performance problems or other modeling related uncertainties (e.g., emission projection factors) on the outcome of the modeled attainment and screening tests

- representativeness of days as characterized by the episode selection analysis (e.g., are all key regimes represented? are days for which attainment is not simulated included among the key regimes/design-value days?)

- other uses of the observational data (e.g., trends analysis)

TRANSPORT ASSESSMENT

The EPA guidance requires that States evaluate their impact on other areas ability to meet the ozone standard. The Charlotte, NC area and Augusta, GA areas are two urban areas close to our state boundaries that have are potential non-attainment areas for the 8-hr ozone standard. The impact of proposed reductions on these areas will be evaluated by using the relative reduction factor base design value test to ensure that reductions also occur in them. Additional areas may be included if a trajectory analysis for the episode show a significant impact on areas other than the two mentioned above.

USE OF MODELING AND CORROBORATIVE EVIDENCE TO DEMONSTRATE ATTAINMENT

The attainment demonstration for each area will require an integrated analysis of the modeling results and any corroborative evidence. The relative "weight" of each will be based on an assessment of the confidence (or degree of uncertainty) in the analysis procedures and results (e.g., data completeness, reliability of the methodology, relevant assumptions, credibility of the results), to the extent this can be established.

10 DOCUMENTATION

A technical support document (TSD) describing the modeling/analysis methods and results will be prepared. A single report will be prepared, however, the results for the individual areas of interest will be presented separately. Preparation of this document is described in this section.

Those portions of the TSD that pertain to the base-case and 2010 future-year baseline modeling will be prepared by SAI. The 2007 and 2012 future-year baseline, sensitivity and control-strategy simulation as well as the remaining section will be prepared by SC DHEC, with guidance and assistance from SAI (as needed).

EPA RECOMMENDED ELEMENTS

Each of the recommended subject areas will be addressed in the final report. These include:

- modeling/analysis protocol
- emissions preparations and results
- air quality/meteorology preparations and results
- performance evaluation for air quality simulation model (and other analyses)
- diagnostic tests
- description of the strategy demonstrating attainment
- data access
- weight of evidence determination
- review procedures used

The purpose of and issues associated with each subject area is summarized in the EPA guidance document (EPA, 1999a).

OUTLINE FOR TECHNICAL SUPPORT DOCUMENT

A draft outline for the final report follows:

Executive Summary (including a discussion of the conceptual description of the 8-hour ozone nonattainment problem for each area of interest). It will include a summary of the detailed information contained in the remainder of the document.

I. Introduction
  A. Background and objectives
  B. Modeling grid specification
  C. Episode selection/simulation periods
  D. Characterization of meteorology and air quality of the modeling episodes

II. Modeling Protocol

III. Base-Case Modeling Emission Inventory Preparation
  A. Emissions data
  B. Overview of emissions processing procedures
  C. Preparation of the area and non-road emission inventory component
  D. Preparation of the mobile-source emission inventory component
  E. Preparation of point-source emission inventory component
  F. Estimation of biogenic emissions
  G. Quality Assurance
  H. Summary of the Modeling Emission Inventories

IV Meteorological Modeling and Input Preparation
  A. Overview of the MM5 meteorological modeling system and application procedures
  B. Presentation of results/model performance evaluation
  C. Preparation of UAM-V ready meteorological fields
  D. Quality assurance

V Air Quality, Land-Use, and Chemistry Input Preparation
  A. Air quality related inputs
  B. Land-use inputs
  C. Albedo/haze/ozone column
  D. Chemistry parameters
  E. Quality assurance

VI Model Performance Evaluation
  A. Initial simulation results
  B. Diagnostic and sensitivity analysis
  C. Summary of base-case model performance for each of the urban areas

VII Future-Year Modeling Exercises (for each of the urban areas)
  A. Future-year emission inventory preparation
  B. Future-year boundary conditions preparation
  C. Future-year baseline simulation results
  D. Emission sensitivity simulation results

- E. Control-strategy simulation results

VIII Attainment Demonstration (this will include a subsection for each area of interest and will be completed based on the attainment demonstration runs following final EPA guidance)
- A. Description of the attainment strategy
- B. Modeled attainment and screening test results
- C. Additional analysis
    - 1. Methods
    - 2. Results
- F. Repeat for each type of additional analysis
- G. Integrated weight of evidence analysis
- H. Transport Assesment

IX Summary of review procedures used

X Data access procedures

References

11 ARCHIVAL/DATA ACQUISTION PROCEDURES

The data, input, and output files for the modeling analysis will be available in electronic format. Interested parties should contact Clay Lawson of SC DHEC for information on how to obtain these files. The modeling tools to be used for this study (with the exception of the BEIS and MOBILE, which can be obtained from EPA or other sources) have been delivered to SC DHEC from SAI.

References

Anthes, R. A., and T. T. Warner. 1978. Development of hydrodynamic models suitable for air pollution and other mesometeorological studies. *Mon. Wea. Rev.,* 106:1045-1078.

BAAQMD. 1998. "Bay Area – North Central Coast Photochemical Modeling Investigation of Ozone Formation and Transfer" available electronically at: http://sparc2.baaqmd.gov/MontereyPrj/MontereyPrj.html.

Deuel, H. P., and S. G. Douglas. 1998. "Episode Selection for the Integrated Analysis of Ozone, Visibility, and Acid Deposition for the Southern Appalachian Mountains." Systems Applications International, Inc., San Rafael, California (SYSAPP-98/07r1).

Deuel, H. P., S. G. Douglas, and C. S. Burton. 1998. "Estimation of Modeling System Noise for Two Applications of the UAM-V Modeling System: One-Hour Ozone, Eight-Hour Ozone, and Ozone Exposure." Systems Applications International, Inc., San Rafael, California (SYSAPP- 98/27).

Douglas, S. G., H. H. Tunggal, G. Mansell, and J. L. Haney. 1998. "Subregional Photochemical Modeling Analysis for Atlanta, Birmingham, and the Eastern Gulf Coast Area: Input Preparation and Model Performance Evaluation." Systems Applications International, Inc., San Rafael, California (SYSAPP-98/43d).

Douglas, S. G., and A. B. Hudischewskyj. 1999a. "Preparation of Non-Emissions Related Inputs for Application of the UAM-V Modeling System to the Western U.S." Systems Applications International, Inc., San Rafael, California (SYSAPP-99/31).

Douglas, S. G., A. R. Alvarez, A. B. Hudischewskyj, and J. L. Haney. 1999b. "Episode Selection Analysis for 1-Hour and 8-Hour Ozone for Potential Non-Attainment Areas in Northern Georgia and Alabama." Systems Applications International, Inc., San Rafael, California (SYSAPP-99-12).

Douglas,S. G., A. R. Alvarez, Y. Wei, A B. Hudischewskyj, R. S. Beizaie, and J. L. Haney. 2001. " UAM-V Modeling Analysis of 8-Hour Ozone for the Gulf Coast Ozone Study." Systems Applications International, Inc., San Rafael, California (in progress)

ENSR. 1993. "Model Code Verification of Air Quality and Meteorological Simulation Models for the Lake Michigan Ozone Study." ENSR Consulting and Engineering, Boston, Massachusetts (Doc. # 4133-001-500).

EPA. 1991a. *Emission Inventory Requirements for Ozone State Implementation Plans.* U.S. Environmental Protection Agency, Research Triangle Park, North Carolina (EPA-450/4-91-010).

EPA. 1991b. *Guideline for Regulatory Application of the Urban Airshed Model*. U.S. Environmental Protection Agency (EPA-450/4-91-013).

EPA. 1992a. *User's Guide for the Urban Airshed Model. Volume IV: User's Manual for the Emissions Preprocessor System 2.0*. U.S. Environmental Protection Agency (SYSAPP-92/059a).

EPA. 1992b. *Procedures for the Preparation of Emission Inventories for Carbon Monoxide and Precursors of Ozone, Volume II: Emission Inventory Requirements for Photochemical Air Quality Simulation Models*. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina (EPA-450/R-92-026).

EPA. 1992c. *Quality Review Guidelines for 1990 Base Year Emission Inventories.* U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina (EPA-454/R-92-007).

EPA. 1999a. *Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS.* U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina (EPA-454/R-99-004) May 1999.

EPA. 1999b. *Emissions Inventory Guidance for Implementation of Ozone and Particulate Matter National Ambient Air Quality Standards (NAAQS) and Regional Haze Regulations.* U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina (EPA-454/R-99-006) April 1999.

Gill, D. O. 1992. "A User's Guide to the Penn State/NCAR Mesoscale Modeling System." NCAR Technical Note, National Center for Atmospheric Research, Mesoscale and Microscale Meteorology Division, Boulder, Colorado (NCAR/TN-381+1A).

Haney, J. L. and others. 1995. "Gulf of Mexico Air Quality Study, Final Report. Volume I: Summary of Data Analysis and Modeling." U.S. Department of the Interior, Minerals Management Service, Gulf of Mexico OCS Region, New Orleans, Louisiana.

Hong, S.-Y., and H.-L. Pan. 1995. Nonlocal boundary layer vertical diffusion in a medium-range forecast model. *Mon. Wea. Rev.,*124:2322-2339.

Kain, J. S., and J. M. Fritsch. 1990. A one-dimensional entraining/detraining plume model and its application in convective parameterization. *J. Atmos. Sci.*, 47, 2784-2802.

Ligocki, M. P., and G. Z. Whitten. 1992. "Modeling Air Toxics with the Urban Airshed Model." Presented at the 85th Annual Meeting of the Air and Waste Management Association, Kansas City, June 1992 (Paper 92-84.12).

Messinger F., and A. Arakawa. 1976. Numerical methods used in atmospheric models. *GARP Publications Series No. 14*, World Meteorological Organization Joint Organizing Committee, 64 pp.

OTAG. 1997. "OTAG Regional and Urban Scale Modeling Workgroup. Modeling Report."

SAI. 1999. 18 March GCOS Presentation. Gulfport, Mississippi.

Stauffer, D. R., and N. L. Seaman. 1990. Use of four-dimensional data assimilation in a limited-area mesoscale model. Part I: Experiments with synoptic scale data. *Mon. Wea. Rev.*, 118, 1250-1277.

Stauffer, D. R., N. L. Seaman, and F. S. Binkowski. 1991. Use of four-dimensional data assimilation in a limited-area mesoscale model. Part II: Effects of data assimilation within the planetary boundary layer. *Mon. Wea. Rev.*, 119, 734-754.

Whitten, G. Z., H. P. Deuel, and J. L. Haney. 1996. "Overview of the Implementation of an Updated Isoprene Chemistry Mechanism in CB4/UAM-V." Systems Applications International, Inc., San Rafael, California (Revised Technical Memorandum, 22 July 1996).